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APPLICATIONS OF RANDOM-CHOICE METHOD  
TO PROBLEMS IN SHOCK AND DETONATION-WAVE DYNAMICS

by

T. Saito and I. I. Glass

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T. Saito and I. I. Glass

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**RANDOM-CHOICE METHOD (RCM)  
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SHARP-FRONTED SHOCKS  
CONTACT SURFACES  
PLANAR AND SPHERICAL SHOCK WAVES****RAREFACTION WAVES  
CONTACT SURFACES  
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Eight applications of the Random-Choice Method (RCM) to the solution of problems in shock and detonation-wave dynamics are presented. It is shown that unlike other numerical methods, the RCM yields sharp-fronted shocks and contact surfaces without resorting to artificial and perhaps erroneous means of predicting their locations. It has been shown by examples that the RCM provides exceptionally high computational accuracy for flows involving planar and spherical shock waves, rarefaction waves and contact surfaces, as well as their interactions. In addition, the RCM can handle flows with detonations and chemical reactions involving.

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the above transition fronts. Owing to the high accuracy of calculated values in  $p$ ,  $\rho$ ,  $u$  and the fact that the constant states are perfectly realized, very complex wave-interaction problems which involve small changes in physical parameters  $p$ ,  $u$ ,  $p$ , can be calculated, such as the reflection of a shock wave from the end wall of a shock tube and the subsequent interactions, or the head-on collision of a shock wave with a rarefaction wave.

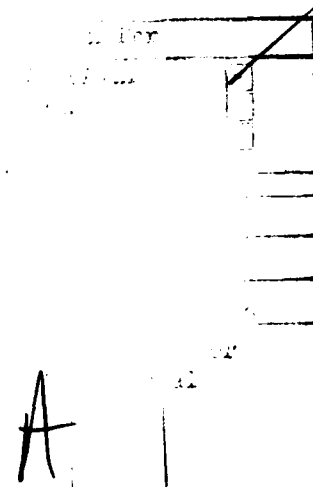
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### Summary

Although successful numerical methods exist for solving problems in shock and detonation-wave dynamics, there is still a real need of developing new techniques where the old methods fail to predict important flow properties. For example, it has recently been shown in Ref. 1 that existing methods fail to predict the interferometrically measured isopycnics in regular and single Mach reflections (let alone complex and double-Mach reflections, for which numerical solutions do not even exist). The purpose of the present report is to present eight applications of the Random-Choice Method (RCM) to the solution of problems in shock and detonation-wave dynamics. It is shown that unlike other numerical methods, the RCM yields sharp-fronted shocks and contact surfaces without resorting to artificial and perhaps erroneous means of predicting their locations, which depend more on art than science. It is also a very useful method in showing such fine points as the birth point of the second shock (implosion) wave at the tail of the rarefaction wave in a spherical explosion.

Despite all these advantages the RCM has yet to be developed to cope with problems such as oblique and spherical shock-wave reflections in order to compute the various isolines (pressure, density and velocity) and compare them with available interferometric or other experimental data. For example, isopycnics are much more sensitive indicators of the accuracy of a given numerical method than a comparison of shock shapes (Ref. 1). Undoubtedly, such applications of the RCM will probably take place in the near future, as the need for such numerical methods now exists.



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### Notation

|            |  |
|------------|--|
| $a$        | speed of sound                                 |
| $C$        | contact surface                                |
| $D$        | speed of detonation wave                       |
| $e$        | total energy per unit volume                   |
| $F$        | function of $V$ , from Eqs. (1), (2) and (34)  |
| $i$        | integer attached to the mesh point in space    |
| $I$        | inhomogeneous term in Eq. (34)                 |
| $K$        | reaction rate                                  |
| $m$        | momentum per unit volume                       |
| $M$        | molecular weight                               |
| $M_l$      | mass flow (fluid enters a wave from the left)  |
| $M_r$      | mass flow (fluid enters a wave from the right) |
| $n$        | integer attached to the mesh point in time     |
| $p$        | pressure                                       |
| $P$        | sampling point                                 |
| $r$        | radial distance                                |
| $S$        | state in Riemann problem; $S_l, S_r, S_*$      |
| $t$        | time   |
| $\Delta t$ | time increment                                 |
| $T$        | temperature                                    |
| $u$        | particle velocity                              |
| $U$        | shock velocity                                 |
| $v$        | solution of Riemann problem, see Eq. (5)       |
| $V$        | solution vector from Eq. (2)                   |
| $w$        | particle velocity relative to wave front       |
| $x$        | space coordinate                               |
| $\Delta x$ | space increment                                |

|            |  |
|------------|--|
| Z          | progress parameter in Eq. (66)                                 |
| a          | 1, 2, 3 for planar, cylindrical, spherical flows, respectively |
| $\gamma$   | specific heat ratio  |
| $\epsilon$ | internal energy per unit mass                                  |
| $\theta$   | random number $-\frac{1}{2} \leq \theta \leq \frac{1}{2}$      |
| $\rho$     | density  |

## 1. INTRODUCTION

Over the past two decades a number of numerical methods have been developed for the solution of flow problems in nonstationary gasdynamics involving transition fronts such as shock waves, rarefaction waves and contact surfaces. Such fronts occur in shock-tube flows, cylindrical and spherical explosions and implosions as well as in combustion with deflagration and detonation. In essence, the set of nonlinear hyperbolic partial differential equations of motion are replaced by a set of finite-difference equations which are numerically integrated for a solution. Owing to truncation errors an implicit artificial viscosity is introduced which spreads the contact-surface and shock-wave fronts over several mesh lengths. This is analogous to the action of real viscosity and heat conduction in spreading the shock transition over several mean-free-paths, and at the contact surface, due to the diffusion of heat and mass, spreading occurs with the square root of time.

Most finite-difference methods when applied to problems with discontinuities such as shock waves produce oscillations behind them. Von Neumann and Richtmyer (Ref. 5) introduced an artificial viscosity pressure term into the Lagrangian form of the gasdynamic equations to get rid of these unwanted oscillations in the solution. Since then various types of explicit or implicit artificial-viscosity terms have been used depending on the type of equations, Lagrangian or Eulerian and the type of finite-difference scheme used. Shock-wave fronts are also smeared by the artificial viscosity term, as well as the truncation error, typically over several mesh points. Moreover the artificial-viscosity term contains an arbitrary parameter which must be determined for each particular problem in order to obtain the best results. For a recent review of the subject see Ref. 4.

Unfortunately, the spreading or smearing of such fronts makes it difficult to know their positions with any precision at a given time. The development of the Random-Choice Method (RCM) by Glimm, Chorin and Sod (Refs. 2, 3 and 6), has made it possible to overcome these difficulties at the expense of some randomness in the paths of these wave fronts. For example, shock waves and contact surfaces are not spread at all and occupy zero zones. Their locations at any time are not exact but their average positions are. The physical profiles of the head and tail of rarefaction waves are perfectly sharp, whereas in other methods they come out rounded. Due to the randomness, the profiles are not smooth but on the average very close to the exact values for the rarefaction wave. In case of a shock-tube flow, the uniform states separated by the contact surface are obtained exactly without oscillations. Boundary conditions are readily handled by the RCM. The time required for the RCM may be two or threefold longer than for the other methods. However, the number of grid points are fewer for the same resolution. Consequently, the computation time can be much faster.

It is known that wave-interaction problems can be analyzed by using the method of characteristics. The solution, in this case, is computed with the aid of a grid of characteristic lines, which is constructed in the course of the computation. This method is used mainly for a detailed description of the flows. For example, the method of characteristics permits one to determine accurately the birth point of secondary shock waves in a flow at the point of intersection of the characteristics of one family. However, if a large number of such shock waves occur, difficulties would be encountered. Accordingly, the method of characteristics is usually applied to problems where the number of discontinuities is small.

The RCM does not resort to any type of finite-difference scheme to obtain the solutions for wave-interaction problems. A set of states at two adjacent mesh points  $i$  and  $(i + 1)$ , at  $t = 0$ , form a Riemann problem (shock-tube problem) with the Euler type of equations of motion, namely, mass, momentum and energy. From the method of characteristics it is known that a Riemann problem has a self-similar solution which consists of four uniform states consisting of the two initial states, two final states, separated by a contact surface and a nonuniform state, the rarefaction wave. All the thermodynamic and dynamic properties can be calculated exactly from an algebraic consideration of the transition relations for shock fronts and rarefaction waves (Ref. 34). After the Riemann problem has been solved, one of the five states is chosen at random. This choice makes it possible to find a solution subsequently, at a time  $\Delta t/2$ , at a random point  $P$ , which is located between the mesh points  $i$  and  $(i + 1)$  as shown in Fig. 1. Although  $P$  is located in state (2), this solution is assigned to mesh point at  $(i + 1/2)$ . It may appear that this is in error since the mesh point is really in state (3) in Fig. 1. However, if we realize that the mesh points are the representatives of elemental regions of the whole flow field,  $(i + 1/2)$  could have been at point  $P$ , i.e., the mesh points are not fixed in physical space. This randomness, on the average, is cancelled out and the correct solution is obtained. Although this sampling procedure gives randomness in the wave positions and the shape of the rarefaction waves, it is in reality acceptable and the calculated values are exact due to the fact that the method is free from truncation errors and artificial viscosity.

Many wave-interaction problems were investigated theoretically and experimentally at UTIAS. Finite-difference schemes with artificial viscosity were used mainly for solving the gasdynamic equations in Eulerian or Lagrangian form. In this report, the RCM is first applied to some of the practical wave-interaction problems. Although the mathematical justification of the RCM has already been shown in Refs. 2 and 3, it is important to check the usefulness and the applicability of the method to practical problems.

So far, the RCM has been applied to planar, cylindrical and spherical flows (Refs. 3 and 6) as well as to combustion flows (Ref. 7). Some very important applications of the RCM would be to pseudostationary oblique shock-wave reflection problems as well as nonstationary cylindrical and spherical shock-wave reflections. This has not been fully accomplished to date.

In Chapter 2, the RCM is described for the sake of completeness. Problems involving different gases with different values of the specific heat ratio  $\gamma$  were not calculated previously using the RCM. In this report the program was modified in order to make it possible to solve problems involving combinations of gases with different values of  $\gamma$ . The procedure is described in Appendix A. Chapter 3 deals with several examples of simple shock-tube flows solved by using the RCM. The results are compared with exact or approximate solutions. Chapter 4 extends Sod's RCM for cylindrical and spherical symmetric flows. Chorin's method for calculating reacting gas flows is also briefly described. The methods are applied to some practical examples, which required a modification of Chorin's program. Discussions and conclusions can be found in Chapter 5, and the program listings are given in Appendix B.

## 2. RANDOM-CHOICE METHOD (RCM)

### 2.1 GENERAL DESCRIPTION OF RCM

The equations for an inviscid non-heat-conducting one-dimensional flow can be written in conservation form (Ref. 3):

$$V_t + F(V)_x = 0 \quad (1)$$

where

$$V = \begin{pmatrix} \rho \\ m \\ e \end{pmatrix} \quad F(V) = \begin{pmatrix} m \\ m^2/\rho + p \\ m(e+p)/\rho \end{pmatrix} \quad (2)$$

and the subscripts indicate differentiation. The total energy per unit volume  $e$ , may be written as

$$e = \rho \epsilon + \frac{1}{2} \rho u^2 \quad (3)$$

Assuming the gas is polytropic, the internal energy per unit mass is given by

$$\epsilon = \frac{1}{\gamma - 1} \frac{p}{\rho} \quad (4)$$

Letting  $\Delta t$  and  $\Delta x$  be time and spatial increments, respectively, the solution of the system of equations, Eq. (1), is to be evaluated at the mesh points  $(i\Delta x, n\Delta t)$ , and  $\{(i + 1/2)\Delta x, (n + 1/2)\Delta t\}$ . Letting  $v_i^n$  approximate  $V(i\Delta x, n\Delta t)$  and  $v_{i+1/2}^{n+1/2}$  approximate  $V\{(i + 1/2)\Delta x, (n + 1/2)\Delta t\}$ , it is necessary to find  $v_{i+1/2}^{n+1/2}$  given  $v_i^n, v_{i+1}^n$ .

Consider an initial value problem for the system of equations given by Eq. (1), with the discontinuous initial data,

$$V(x, n\Delta t) = \begin{cases} v_{i+1}^n, & x \geq (i + 1/2)\Delta x \\ v_i^n, & x < (i + 1/2)\Delta x \end{cases} \quad (5)$$

then Eq. (1) together with Eq. (5) is called a Riemann problem. A method for solving such a Riemann problem will be described in detail in the next section. Let  $v(x, t)$  denote the solution of this Riemann problem and let  $\theta_n$  be a value of the random variable  $\theta$  equidistributed in  $[-1/2, 1/2]$ . Then define  $v_{i+1/2}^{n+1/2}$  by the solution of the Riemann problem at the point  $\{(i + 1/2 + \theta_n)\Delta x, (n + 1/2)\Delta t\}$

$$v_{i+1/2}^{n+1/2} = v \left\{ \left( i + \frac{1}{2} + \theta_n \right) \Delta x, \left( n + \frac{1}{2} \right) \Delta t \right\} \quad (6)$$

namely, at each time step the solution is first approximated by a piecewise constant; i.e., Riemann problems are formed with respect to each pair of every other mesh points. Time is then advanced exactly, and the new values on the mesh points in between those used to construct the Riemann problems are chosen by sampling (Fig. 1). The justification of this method for solving the system of equations, Eq. (1), can be found in Refs. 2 and 3.

## 2.2 SOLUTION OF A RIEMANN PROBLEM

The method of solving a Riemann problem is now described. Consider the system of equations given by Eq. (1) with the initial data,

$$V(x, 0) = \begin{cases} S_r = (\rho_r, u_r, p_r) & x \geq 0 \\ S_l = (\rho_l, u_l, p_l) & x < 0 \end{cases} \quad (7)$$

The solution at later times will consist of three states; a left state  $S_l$ , a right state  $S_r$ , a middle state  $S_*$  with  $u = u_*$ ,  $p = p_*$  and  $\rho = \rho_*$  separated from  $S_l$  and  $S_r$  by waves,  $W_r, W_l$ , which may be either shock waves or rarefaction waves. A contact surface ( $dx/dt = u_*$ ) separates the gas initially at  $x < 0$  from the gas initially at  $x \geq 0$ . The values of  $u$  and  $p$  are continuous across the contact surface while  $\rho$  and other thermodynamic quantities, in general, are not. The contact surface divides  $S_*$  into two regions with differing values of densities  $\rho_{*l}$  and  $\rho_{*r}$ , but equal constant values of  $u_*$  and  $p_*$  (Fig. 2).

Using Godunov's iterative method modified by Chorin and Sod (Refs. 3 and 6)  $\rho, u, p$  at the sample point  $P(\theta \Delta x, 1/2 \Delta t)$ ,  $-1/2 \leq \theta \leq 1/2$ , are determined as follows: Define the quantity

$$M_r = (p_r - p_*) / (u_r - u_*) \quad (8)$$

If the right wave is a shock wave, using the jump condition across the shock wave, we obtain

$$M_r = -\rho_r(u_r - U_r) = -\rho_{*r}(u_* - U_r) \quad (9)$$

where  $U_r$  is the velocity of the right shock wave. From the Rankine-Hugoniot conditions one obtains

$$M_r = (\rho_r p_r)^{1/2} \phi_1 \left( \frac{p_*}{p_r} \right), \quad \frac{p_*}{p_r} \geq 1 \quad (10)$$

where

$$\phi_1(\eta) = \left( \frac{\gamma+1}{2} \eta + \frac{\gamma-1}{2} \right)^{1/2} \quad (11)$$

If the right wave is a rarefaction wave, using the isentropic law  $p\rho^{-\gamma} = \text{constant}$  and the constancy of the right Riemann invariant  $\Gamma_r = 2(\gamma p/\rho)^{1/2}/(\gamma-1) - u$ , we find

$$M_r = (\rho_r p_r)^{\frac{1}{2}} \phi_2 \left( \frac{p_*}{p_r} \right), \quad \frac{p_*}{p_r} < 1 \quad (12)$$

where

$$\phi_2(\eta) = \frac{\gamma - 1}{2\gamma^{\frac{1}{2}}} \frac{1 - \eta}{1 - (\gamma - 1)/2\gamma} \quad (13)$$

The function

$$\phi(\eta) = \begin{cases} \phi_1(\eta) & \eta \geq 1 \\ \phi_2(\eta) & \eta < 1 \end{cases} \quad (14)$$

is continuous at  $\eta = 1$ , with  $\phi(1) = \phi_1(1) = \phi_2(1) = \gamma^{\frac{1}{2}}$ . Similarly, we define

$$M_\ell = (p_\ell - p_*) / (u_\ell - u_*) \quad (15)$$

If the left wave is a shock wave,

$$M_\ell = \rho_\ell (u_\ell - U_\ell) = \rho_{*\ell} (u_* - U_\ell) \quad (16)$$

where  $U_\ell$  is the velocity of the left shock wave. As on the right,

$$M_\ell = (\rho_\ell p_\ell)^{\frac{1}{2}} \phi \left( \frac{p_*}{p_\ell} \right) \quad (17)$$

where  $\phi(\eta)$  is defined as in Eqs. (11), (13) and (14). Eliminating  $u_*$  from Eqs. (8) and (15), we obtain

$$p_* = \frac{u_\ell - u_r + p_r/M_r + p_\ell/M_\ell}{1/M_r + 1/M_\ell} \quad (18)$$

Equations (18), (17) and (10) or (12) are three equations with three unknowns  $p_*$ ,  $M_\ell$  and  $M_r$ . These considerations lead to the following iteration procedure: Choose a starting value  $p_*^0$  (or  $M_r^0$ ,  $M_\ell^0$ ), and then compute  $M_r^{v+1}$ ,  $M_\ell^{v+1}$ ,  $p_*^{v+1}$  ( $v \geq 0$ ) using

$$\tilde{p}^v = (u_\ell - u_r + p_r/M_r^v + p_\ell/M_\ell^v) / (1/M_r^v + 1/M_\ell^v) \quad (19)$$

$$p_*^{v+1} = \max(\epsilon_1, \tilde{p}^v) \quad (20)$$

$$M_r^{v+1} = (\rho_r p_r)^{\frac{1}{2}} \phi(p_*^{v+1}/p_r) \quad (21)$$

$$M_\ell^{v+1} = (\rho_\ell p_\ell)^{\frac{1}{2}} \phi(p_*^{v+1}/p_\ell) \quad (22)$$



Since there is no guarantee that  $\tilde{p}$  remains  $\geq 0$ , Eq. (20) is needed. The iteration is stopped when

$$\max(|M_\ell^{v+1} - M_\ell^v|, |M_r^{v+1} - M_r^v|) \leq \epsilon_2$$

Then put

$$M_\ell = M_\ell^{v+1}, M_r = M_r^{v+1}, p_* = p_*^{v+1}$$

Chorin picked the value of  $\epsilon_1 = 10^{-6}$ ,  $\epsilon_2 = 10^{-6}$  in this iteration cycle. To start this iteration cycle either  $M_r$  and  $M_\ell$  or  $p_*$  is needed. From the point of view of computation time, the efficiency of the RCM depends on how fast this iteration converges. Chorin obtained better results putting

$$p_*^0 = (p_\ell + p_r)/2$$

as a starting value of the procedure than following the starting scheme suggested by Godunov (Ref. 8).

Godunov mentioned that the iteration may fail to converge in the presence of a strong rarefaction wave. This problem can be overcome by the following variant of Godunov's procedure. If the iteration has not converged after  $J$  iterations, Eq. (20) is replaced by

$$p_*^{v+1} = \zeta \max(\epsilon_1, \tilde{p}^v) + (1 - \zeta)p_*^v$$

with  $\zeta = \zeta_1 = \frac{1}{2}$ . In general  $\zeta$  will be reset

$$\zeta = \zeta_j = \frac{1}{2} \zeta_{j-1}$$

after  $jJ$  iteration,  $j = 1, 2, 3, \dots$ . Chorin noted that the cases  $j > 2$  had never been encountered and the number of iterations required fluctuated between 2 and 10, except at a very few points.

Knowing  $M_\ell$ ,  $M_r$ ,  $p_*$ , Eqs. (8) and (15) give

$$u_* = (p_\ell - p_r + M_\ell u_\ell + M_r u_r) / (M_\ell + M_r) \quad (23)$$

### 2.3 SAMPLING PROCEDURE

Having a solution in the middle state  $S_*$ , the next step is to determine the solution at each mesh point by sampling. There are four basic cases to be sampled.

- 1) The sampling point  $P = (\theta \Delta x, \frac{1}{2} \Delta t)$  lies to the right of the contact surface whose inverse slope in the  $(x, t)$ -plane is  $(dx/dt) = u_*$ , and the right wave is a shock wave, i.e.,

$$\theta \Delta x \geq u_* \Delta t / 2 \text{ and } p_* \geq p_r$$

As mentioned before  $\theta$  is a random number uniformly distributed over the range of  $[-\frac{1}{2}, \frac{1}{2}]$ .

- 2) The sampling point  $P$  lies to the left of the contact surface and the left wave is a rarefaction wave, i.e.,

$$\theta \Delta x < u_* \Delta t / 2 \text{ and } p_* < p_\ell$$

- 3) The sampling point P lies to the left of the contact surface and the left wave is a shock wave, i.e.,

$$\theta \Delta x < u_* \Delta t / 2 \text{ and } p_* \geq p_\ell$$

- 4) The sampling point P lies to the right of the contact surface and the right wave is a rarefaction wave, i.e.,

$$\theta \Delta x > u_* \Delta t / 2 \text{ and } p_* < p_r$$

In what follow  $\bar{\rho}$ ,  $\bar{u}$ ,  $\bar{p}$  denote the sampled solution, and now how they are determined is explained for each case.

Case 1) From Eq. (9), the velocity of the right shock wave  $U_r$  can be obtained as

$$U_r = u_r + M_r / \rho_r \quad (24)$$

If the sampling point P lies to the right of the shock-wave line  $dx/dt = U_r$ , region 1 in Fig. 3,

$$\bar{\rho} = \rho_r, \bar{u} = u_r, \bar{p} = p_r$$

If the sampling point P lies to the left of the shock wave, region 2 in Fig. 3,

$$\bar{\rho} = \rho_{*r}, \bar{u} = u_*, \bar{p} = p_*$$

where  $\rho_{*r}$  is obtained from Eq. (9) as

$$\rho_{*r} = -M_r / (u_* - U_r) \quad (25)$$

Case 2) The rarefaction wave is bounded on the left by the line  $dx/dt = u_\ell - a_\ell$ , and on the right by  $dx/dt = u_* - a_*$ , where  $a_\ell$  and  $a_*$  are the sound velocities in the states  $S_\ell$  and  $S_*$ , respectively;  $a_\ell$  is given as

$$a_\ell = \sqrt{\gamma_\ell p_\ell / \rho_\ell} \quad (26)$$

and  $a_*$  can be found by using the Riemann invariant  $\Gamma_\ell = \text{constant}$ ,

$$2a_*/(\gamma_\ell - 1) + u_* = 2a_\ell/(\gamma_\ell - 1) + u_\ell = \Gamma_\ell$$

If the sampling point P lies to the left of the head of the rarefaction wave,  $dx/dt = u_\ell - a_\ell$ , region 5 in Fig. 3,

$$\bar{\rho} = \rho_\ell, \bar{u} = u_\ell, \bar{p} = p_\ell$$

If the sampling point P lies to the right of the tail of the rarefaction wave,  $dx/dt = u_* - a_*$ , region 3 in Fig. 3, set

$$\bar{\rho} = \rho_{*\ell}, \bar{u} = u_*, \bar{p} = p_*$$

where  $\rho_{*l}$  is calculated using the isentropic relation  $p\rho^{-\gamma} = A$  (constant), as

$$\rho_{*l} = (p_*/A)^{1/\gamma_l} \quad (27)$$

The value of  $A$  can be calculated in the state  $S_l$  as

$$A = p_* \rho_{*l}^{-1/\gamma_l} \quad (28)$$

If the sampling point  $P$  lies inside the rarefaction wave, region 4 in Fig. 3, the slope of the characteristic  $dx/dt = u - a$  is equated to the slope of the line connecting the origin and  $P$ , to obtain

$$\bar{u} - a = 2\theta\Delta x/\Delta t \quad (29)$$

Also,

$$2a/(\gamma_l - 1) + \bar{u} = 2a_l/(\gamma_l - 1) + u_l = r_l \quad (30)$$

Solving Eqs. (29) and (30), obtain

$$\bar{u} = \frac{2}{\gamma_l + 1} \left( \frac{2\theta\Delta x}{\Delta t} + a_l + \frac{\gamma_l - 1}{2} u_l \right) \quad (31)$$

Since  $a = (\gamma_l \bar{p}/\bar{\rho})^{1/2}$  and  $\bar{p} = A \bar{\rho}^{\gamma_l}$

$$\bar{\rho} = (a^2/\gamma_l A)^{1/(\gamma_l - 1)} \quad (32a)$$

$$\bar{p} = A \bar{\rho}^{\gamma_l} \quad (32b)$$

Cases 3 and 4 are mirror images of cases (1) and (2) and the same arguments are applied.

#### 2.4 PRODUCTION OF RANDOM NUMBERS

The choice of a series of random numbers  $\theta_n$  ( $n = 1, 2, \dots$ ) determines the behaviour of the solution. If  $\theta$  is close to  $-1/2$ , the values in the left state  $S_l$  propagate to the right to  $\{(i + 1/2)\Delta x, (n + 1/2)\Delta t\}$ , while, if  $\theta$  is close to  $1/2$ , the values in the right state  $S_r$  propagate to the left. Therefore it is important to choose  $\theta_n$  in such a way that they tend to be equally distributed over  $[-1/2, 1/2]$  as soon as possible.

Chorin noted that it is unreasonable to choose a new value of  $\theta$  for each mesh point  $i$ , at each time level  $n$ , since there is a finite probability that a given state  $S$  will propagate in both directions. Chorin overcame this problem choosing a new value of  $\theta$  once for each time level rather than assigning a new value of  $\theta$  for each  $i$  and  $n$ . Chorin further improved the method by making the sequence of random numbers  $\theta_n$ , reach equidistribution over  $[-1/2, 1/2]$  at a faster rate. This is done by combining a random number  $\theta_n$  chosen from the range of  $[-1/2, 1/2]$  and a pseudorandom number  $k_n$ .

Let  $m_1$  and  $m_2$  be two mutually prime integers ( $m_1 < m_2$ ) then consider the sequence of integers,

$$k_{n+1} = (m_1 + k_n) \pmod{m_2}$$

where  $k_0$  is given,  $k_0 < m_2$ . This will produce a series of pseudorandom numbers. For example, if  $k_0 = 1$ ,  $m_1 = 3$ ,  $m_2 = 7$ , then  $k_1, k_2, k_3, \dots$  will be a repetition of a series of integers, 4, 0, 3, 6, 2, 5, 1. If we consider the following sequence:

$$\theta'_n = \frac{k_n + (\theta_n + 1/2)}{m_2} - \frac{1}{2} \quad (n = 1, 2, \dots)$$

$\theta'_n$  will be also in the range of  $[-1/2, 1/2]$ . This modified sequence of random numbers  $\theta'_n$  is employed in the program. The advantages of using this sequence  $\theta'_n$  is described in detail in Ref. 3.

## 2.5 BOUNDARY CONDITIONS

Consider a solid-wall boundary at  $x = b$ , with the fluid to the left. The boundary conditions are imposed on the grid point closest to  $x = b$ , say  $i_0 \Delta x$ . A pseudo right state  $S_r$  at  $(i_0 + 1/2) \Delta x$  is created by setting

$$\begin{aligned} \rho_{i_0+1/2} &= \rho_{i_0-1/2} \\ u_{i_0+1/2} &= u_{i_0-1/2} \\ P_{i_0+1/2} &= P_{i_0-1/2} \end{aligned} \quad (33)$$

In this manner, waves can be reflected at a solid boundary.

## 2.6 TREATMENT OF CONTACT SURFACES

The Random-Choice Method was not applied to flow problems having combinations of gases with different specific heat ratios. In this report the program was modified to handle such problems, thereby enlarging the applicability of the RCM. The position of contact surfaces are determined during sampling procedure and consistent with the RCM. The details are given in Appendix A.

## 3. NUMERICAL RESULTS FOR PLANAR WAVE INTERACTIONS

The purpose of this section is to show how well the RCM works for nonstationary wave-interaction problems by using several illustrative examples. Many examples of interactions of shock waves, rarefaction waves, contact surfaces and with solid boundaries are given in Refs. 9 and 10.

In order to illustrate the usefulness of the RCM, the following examples were calculated:

1. Reflection of shock wave from end wall of a shock tube and subsequent interactions.

2. Head-on collision of a shock wave with a rarefaction wave.
3. Head-on collision of two rarefaction waves.
4. Contact-surface tailoring.
5. Shock-refraction problem at a stationary contact layer.
6. Shock-wave propagation in a varying-density field.

### 3.1 REFLECTION OF SHOCK WAVE FROM END WALL OF A SHOCK TUBE AND SUBSEQUENT INTERACTIONS.

The initial conditions were set in such a way that we could compare the results obtained using the RCM with those obtained by Gurke and Schwarzkopf (Ref. 11), i.e.,

diaphragm pressure ratio :  $P_{41} = 27.0$

test gas - air :  $\gamma_1 = 1.40$

driver gas - air :  $\gamma_4 = 1.40$

Figure 4 was drawn from the data in Ref. 11. Since these results were obtained with the method of characteristics and there is no interactions between shock waves and rarefaction waves, the solutions obtained here are exact. Figure 5 shows our results obtained with the RCM for a mesh number of 720 along the axis of the shock tube. Only the region close to the end wall is displayed. Since this method does not make use of an artificial viscosity, shock waves and contact surfaces remain perfectly sharp. Owing to this outstanding feature, we can recognize as many as 68 different regions without difficulty in this particular case. The exact wave trajectories in Fig. 4 are superimposed in Fig. 5 as solid lines for ready comparison with the present results. It can be seen that the agreement in wave positions is excellent. At  $t \approx 2.5$  ms, the error in the position of the contact surface is about 6 mesh sizes, and appears to be the largest error in the region where the exact solution is presented for comparison. This error corresponds to about 0.8% of the whole mesh number, i.e., 1.3 cm for a 180-cm long shock tube. The discrepancy of the wave positions from the exact solution depends on the mesh size and was about 3% when the mesh number was 180. In Table 1, values of pressure  $P$ , density  $\rho$ , and particle velocity  $u$ , obtained by the present method are compared with the exact solution for each region. In these regions, the numerical errors in both pressure and density are of the order of  $10^{-4}$ . Although they tend to increase as time goes on, their magnitudes are small enough to consider the numerical values as exact. In Table 2 numerically obtained values of  $P$ ,  $\rho$ ,  $u$  are listed for all the regions which appear on Fig. 5. In Fig. 5 and Table 2 we see that the flow patterns get more and more complex and also, as one can expect, the changes in values of  $\rho$ ,  $u$ ,  $P$  become smaller. For example, in regions 67 and 68, across them the changes in pressure and density are from 24.690 to 24.694, and from 8.719 to 8.721, respectively.

All the numerical computations were done using an IMB 370. It took 77.78 min to calculate this example with 720 mesh numbers and 1600 time steps. This fairly long computation time includes the time spent to calculate the solutions

at mesh points far from the end wall in which, however, there is no immediate interest. Therefore, if we could simulate wave interactions only in the region close to the end wall, significant computation time could be saved.

This can be done as follows. First, calculate the values of  $\rho$ ,  $u$ ,  $p$  in the regions 2 and 3 for the given initial conditions by using either Rankine-Hugoniot relations or this numerical method. Then distribute states 1, 2 and 3 as the initial conditions over the mesh points and by removing the boundary conditions at the other end wall of the shock tube so that no reflected rarefaction wave is generated there. This corresponds to a shock tube with an infinitely long high-pressure section. In the same way, one can always simulate only those wave interactions that one is interested in, that is, a larger dynamic range for the wave interactions for the same mesh number. It took 3.19 minutes to calculate the same problem with a mesh number of 180 and 300 time steps, or from  $t = 0$  to  $t = 3.6$  ms in this particular case. Many wave interaction patterns are seen in Fig. 5, such as the overtaking of two similarly facing shock waves, the head-on collisions among shock and rarefaction waves, the interaction of a shock or rarefaction wave with a contact surface. Some of these basic interaction problems were simulated in detail and will be discussed subsequently.

### 3.2 HEAD-ON COLLISION OF A SHOCK WAVE WITH A RAREFACTION WAVE

This interaction problem was investigated by Gould (Ref. 12) both analytically and experimentally. The initial conditions provided for a shock strength  $p_{10}$ , and rarefaction strength  $p_{20}$  of  $p_{10} = 1.96$  and  $p_{20} = 0.549$ . This is achieved by putting the left diaphragm pressure ratio  $p_{70} = 4.15$  and the right diaphragm pressure ratio  $p_{08} = 3.26$  with  $\gamma = 1.40$ .

Figure 6 shows the resulting wave system for this case. As a result of the head-on collision of a forward facing shock wave (fluid particles enter the wave from the right) and a backward facing rarefaction wave (fluid particles enter the wave from the left), there appears a forward facing transmitted shock wave and a backward facing rarefaction wave. Since the shock wave increases in strength continuously during the interaction with the rarefaction wave, each fluid particle crossing the shock wave in this period of time will experience a different entropy jump thereby forming a contact layer or region. Consequently, the region between the transmitted shock wave and the transmitted rarefaction wave consists of two new uniform regions (3), (4) and a contact region. (Note that secondary interactions of characteristics within the contact layer have been neglected.) Pressure  $p$ , and particle velocity  $u$ , are the same for regions (3) and (4), but density  $\rho$ , temperature  $T$ , and entropy  $S$ , are different. The exact values of  $\rho$ ,  $u$ ,  $p$  in the regions (3) and (4) can be determined analytically. The wave trajectories, however, in the interaction region were determined by Gould in detail, as outlined in Ref. 12. In Fig. 6, the wave trajectories were obtained only by averaging the initial and final stage of the interaction without the detailed method of Gould. The results (circled data) obtained by the RCM are superimposed on those obtained by Gould in Fig. 6. In Table 3, the computed values of  $\rho$ ,  $u$ ,  $p$  are compared with those obtained by Gould. As we can see, the calculated values are correct to at least the first four digits and the error is of the order of  $10^{-4}$ . The agreement in the wave trajectories is also very good and the error is about 1% at the most.

The computation was carried out with 180 spatial mesh points and it took 0.72 minutes to proceed through 82 time steps, which was long enough to simulate the interaction process appearing in Fig. 6.

In Table 3, as mentioned before, the pressure  $p$  and particle velocity  $u$  are the same for regions (3) and (4) but the density  $\rho$  is different. The density change across the contact region is as small as 0.19% of its absolute value.

### 3.3 HEAD-ON COLLISION OF TWO RAREFACTION WAVES.

This problem was solved by Steketee (Ref. 13). The computer simulation was done by assuming an experiment using a two-diaphragm shock tube. Initially the center part, which is separated by two diaphragms both from the left part and right part of the shock tube, is filled with a gas at higher pressure than the other two sections so that, after the two diaphragms are ruptured, rarefaction waves propagate into this center section and collide. The assumed initial conditions for the numerical calculations were

|                 |                                       |                  |                  |
|-----------------|---------------------------------------|------------------|------------------|
| left section:   | Ar ( $\gamma = 1.6667$ ):             | $p = 0.088118$ , | $\rho = 1.7457$  |
| centre section: | H <sub>2</sub> ( $\gamma = 1.4000$ ): | $p = 1.0000$ ,   | $\rho = 1.0000$  |
| right section:  | Ar ( $\gamma = 1.6667$ ):             | $p = 0.024793$ , | $\rho = 0.49119$ |

This will give the forward-facing rarefaction wave strength  $P_{20}$ , of 0.59498 and the backward-facing rarefaction wave strength  $p_{10}$ , of 0.39945.

After the interaction, a uniform state appears between the two transmitted rarefaction waves. Unlike the previous case the interaction process is isentropic and no contact region will be produced. The values of  $p$ ,  $u$ ,  $p$  in this uniform region can be determined exactly. The exact values and the results obtained from the RCM are displayed in Table 4. Again the errors in this calculated values are very small. Figure 7 is the  $(x, t)$ -diagram for this interaction. The circles are the results obtained using the RCM and lines are those obtained by the method of characteristics (Ref. 13). The agreement is, in general, good especially before the interaction. The agreement of boundaries between the state (3) and transmitted rarefaction waves do not look too good. This relatively large error, typically about 3%, includes the error associated with the method of characteristics and we can expect smaller errors for the RCM itself. On the region of penetration, the characteristic lines are no longer straight, and their trajectories had to be determined graphically dividing the rarefaction waves into small segments. In Fig. 7, trajectories of characteristic lines were obtained by dividing both rarefaction waves into four segments. As far as the wave trajectories are concerned, since it is not practical to divide the rarefaction fans into too many segments, the method of characteristics is also approximate in this problem.

It took 1.72 min to compute 180 time steps with 180 spatial mesh numbers.

### 3.4 CONTACT-SURFACE TAILORING

In general, when a shock wave reflects at the channel end wall and collides with the oncoming contact surface, the shock wave is transmitted and either a shock wave or a rarefaction wave is reflected. However, by choosing the initial conditions properly, they provide a contact surface such that the reflected wave is a Mach wave. As a result, the gas from the end wall to the contact surface remains in a uniform or tailored state. Figure 8 shows such a condition where the wave between states (5) and (7) is a Mach wave. Since state (5) is stationary ( $u_5 = 0$ ), states (7) and (8) are also stationary ( $u_7 = u_8 = 0$ ) and the contact surface is brought to a complete stop. When the flow is tailored, one can get a relatively long test time in the stationary region, which is very useful for aerodynamic and chemical-kinetic studies.

Tailoring in this case was produced by using two different gases with different specific heat ratios. This problem requires a high degree of accuracy for a solution and becomes very difficult for those methods with a finite difference scheme in which contact surfaces cannot be well defined. Given the initial test gas conditions, the diaphragm pressure ratio  $p_{41}$  and the composition of the driver gas can be determined by assuming the incident shock strength  $p_{21}$  (Ref. 14). Using argon as a test gas ( $\gamma_1 = 1.667$ ,  $M_1 = 39.94$ ), the diaphragm pressure ratio  $p_{41}$  and the molecular weight of the driver gas (assuming a diatomic gas with  $\gamma_4 = 1.400$ )  $M_4$ , were calculated for  $p_{21} = 12.30$ . The calculated results give values for  $p_{41} = 58.21$  and  $M_4 = 7.251$  ( $\rho_{41} = 10.57$ ). This driver gas can be made by mixing 79.87% of hydrogen and 20.13% of nitrogen, for example. The calculated values and the results obtained by the RCM are compared in Table 5 and in Fig. 8. It is seen the calculated values of  $\rho$ ,  $u$ ,  $p$  in each region are very accurate. The wave trajectories are in good agreement until the moment when the incident shock wave reflects from the end wall, where it leaves with slight delay, causing a spatial error of about 2%. Although it fluctuates back and forth one mesh size due to the randomness of the sampling procedure, the contact surface stopped after its interaction with the reflected shock wave, as expected.

It took 2.38 min to simulate 250 time steps with 180 mesh numbers.

### 3.5 SHOCK REFRACTION PROBLEM AT A STATIONARY CONTACT LAYER.

The interaction of a shock wave and a stationary contact surface was investigated analytically by Bitondo, Glass and Patterson (Ref. 15) and experimentally by Ford and Glass (Ref. 16). After normal reflection of a shock wave at a stationary contact surface, there are two possible cases; a transmitted shock wave, contact surface and reflected rarefaction wave, or a transmitted shock wave, contact surface and reflected shock wave, depending on the incident shock strength and the initial internal energy ratio (acoustic impedance) across the contact surface. Putting a helium layer in air (Air || He || Air), both cases occur at the two contact surfaces. In the simulation, the incident shock strength was 3.700. In this case, at the left contact surface  $C_l$  (Air || He) a reflected rarefaction wave appears and at the right contact surface  $C_r$  (He || Air) a reflected shock wave results. The solution for  $\rho$ ,  $u$ ,  $p$  can be determined exactly and they are compared with the computed results in Table 6. The interactions are shown in Fig. 9 with the results computed by RCM. In this particular case, the shock strength was attenuated after passing through the helium layer, from a pressure ratio of 3.700 to 2.971. For further details see Ref. 16, where it is shown that other interactions soon amplify the shock wave to nearly its original strength. The order of errors both in the calculated values in the flow variables and in the wave positions are the same as the previous examples. It took 0.70 min to calculate 140 time steps of this problem with 180 mesh numbers.

### 3.6 SHOCK-WAVE PROPAGATION IN A VARYING-DENSITY FIELD.

When a shock wave propagates in a gas which is stationary but has a certain density distribution in the direction of the wave propagation, the shock wave changes its propagation speed and strength. For example, by cooling a vertical-channel end-wall the test gas remains at constant pressure but has a nonuniform density.

Simulation was done with the following initial conditions. The driver gas was air ( $\gamma_4 = 1.400$ ) and test gas was helium ( $\gamma_1 = 1.667$ ). The density distribution is uniform in the driver section. In the test section, it increases linearly such that  $\rho$  at the end wall is fourfold  $\rho_1$  at the diaphragm position. This density change can be obtained by cooling the test gas from 298° K at the diaphragm to 74.5° K at the end wall. The initial diaphragm pressure ratio was taken as  $p_{41} = 30$ .



The results are displayed in Fig. 10. In this particular case, the shock strength increases from  $p_{21} = 2.24$ , at the moment when the diaphragm was ruptured, to  $p_{21} = 3.17$ , when the shock wave has propagated to the end wall of the shock tube. Correspondingly, the local shock Mach number is also increased. However, since the local speed of sound is reduced due to the density increase (temperature decrease);  $a \propto \sqrt{1/\rho}$ , the propagation speed of the shock wave is reduced. The particle velocities are also decreased. The wave diagram is shown in Fig. 11, where the exact solution for the case when the density  $\rho$  is initially uniform, is superimposed for comparison. As expected, the shock wave and contact surface decelerate. It took 0.503 min to calculate 200 time steps with 100 mesh numbers. It is worthwhile mentioning that this example is difficult to handle using other numerical methods. Technically, the difficulty arises from trying to keep the region ahead of the shock wave stationary until its arrival in a finite difference scheme. The method of characteristics also has difficulties to treat this problem since all the characteristics inside the nonuniform region are not straight.

#### 4. EXTENSIONS OF RANDOM CHOICE METHOD

##### 4.1 ONE-DIMENSIONAL SYMMETRIC FLOW

##### 4.1.1 GENERAL DESCRIPTION

Sod developed a method of calculating one-dimensional symmetric flows such as cylindrical and spherical shock waves by combining the RCM with operator splitting. He gives some numerical results on converging shock wave problems in Ref. 6. Here, Sod's method will be applied to a spherical-explosion problem and the results will be compared with some results obtained by Brode (Ref. 26) using the artificial-viscosity method. The equations for an inviscid, non-heat-conducting, radially-symmetric flow can be written in vector form (Ref. 6):

$$V_t + F(V)_t = -I(V) \quad (34)$$

where

$$V = \begin{pmatrix} \rho \\ m \\ e \end{pmatrix} \quad F(V) = \begin{pmatrix} m \\ m^2/\rho + p \\ m(e+p)/\rho \end{pmatrix} \quad I(V) = (\alpha-1) \begin{pmatrix} m/r \\ m^2/\rho r \\ m(e+p)/\rho r \end{pmatrix}$$

where  $\alpha = 2$ , for cylindrical symmetry,  $\alpha = 3$ , for spherical symmetry and  $\alpha = 1$ , corresponds to planar cases described in Chapter 2.

Exact solutions exist for point-source explosions in the limiting case when the primary shock wave is infinitely strong (or implosions) where the pressure in front of the shock wave is negligible, by comparison to that behind it, or in the acoustic limit, when the shock is very weak (i.e., entropy changes are negligible) (Refs. 17 to 25). Although such solutions are useful whenever they are applicable, they cannot be applied to real problems of finite sources when the shock waves are neither strong nor weak. These solutions do not predict the important features of the flow that exists in an actual case such as the second shock wave and wave interactions in the vicinity of the contact surface. To obtain these features, Eq. (34) must be solved. In general, there are two major difficulties in solving Eq. (34):

- 1) A singularity exists at  $r = 0$ .

- 2) The momentum equation [the second component of Eq. (34)] cannot be expressed in conservation form.

Consequently, Eq. (34) has to be solved numerically. Brode (Refs. 26 - 28) was able to numerically integrate the nonlinear (inhomogeneous) partial differential equations, Eq. (34), for a number of important flow problems involving spherical explosions. Payne (Ref. 29) solved the case of a cylindrical implosion by using a similar method. Lapidus (Ref. 30) computed a cylindrical-implosion problem in Cartesian co-ordinate in two space dimensions. Although these methods have been used successfully to explain physical phenomena, they have inherent disadvantages in that the use of artificial viscosity smears out the wave fronts over several mesh numbers and to find their exact location becomes more of an art than a science.\* By using Sod's method such difficulties including 1) and 2) are eliminated completely.

#### 4.1.2 SOD'S METHOD.

In Sod's method, the first step is to remove the inhomogeneous term  $-I(V)$  from Eq. (34), using the method known as operator splitting. Thus the system

$$V_t + F(V)_x = 0 \quad (35)$$

is solved. In this system, the momentum equation can be expressed in conservation form and the RCM, described in Chapter 2, can be used to obtain solutions. Once the system of equations, Eq. (35), has been solved, the system of ordinary differential equations given by

$$V_t = -I(V) \quad (36)$$

is solved in turn.

In the program, Eq. (36) is solved using a Cauchy-Euler scheme by utilizing the solutions of Eq. (35),  $\bar{V}$ , to determine the inhomogeneous term  $-I$  in Eq. (36), namely, the system Eq. (36) is approximated by

$$(V_i^{n+1} - V_i^n) / \Delta t = -I(\bar{V}_i^{n+1})$$

or

$$V_i^{n+1} = V_i^n - \Delta t I(\bar{V}_i^{n+1}) \quad (37)$$

Since the solutions for the system Eq. (35) are only obtained at intermediate points and the scheme of Eq. (37) does not require values at  $r = 0$ , the singularity at the axis is eliminated. The boundary conditions are properly imposed on Eq. (35), as described in Sec. 2 - 5. There is no need to put boundary conditions on Eq. (36), since it is solved only at intermediate points.

#### 4.1.3 EXPLOSION OF A PRESSURIZED HELIUM SPHERE.

A set of experimental results for the explosion of pressurized glass spheres

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\*The reader will find a fuller discussion in Ref. 38.

filled with air or helium into air may be found in Refs. 26, 31 and 32. As an example of Sod's method, one of the experimental conditions for a helium explosion was used as initial conditions for the numerical analysis,

$$\begin{aligned} \text{diaphragm pressure ratio: } p_{41} &= 18.25 \\ \text{diaphragm density ratio: } \rho_{41} &= 2.523 \\ \text{initial particle velocities: } u_1 &= u_4 = 0 \end{aligned} \quad (38)$$

At the instant of rupture, the planar-wave conditions apply, giving a shock strength  $p_{21} = 6.497$ . The shock wave then decelerates until it becomes a sound wave. The contact surface decelerates and its motion becomes oscillatory. The rarefaction-wave head moves at constant speed and reflects at the origin where its motion becomes complex. The tail of the rarefaction wave accelerates and an implosion (second shock) wave originates on it.

Equation (34) may be reexpressed in the following form by using the method of characteristics (Ref. 25).

Along a right running characteristics or P-wave,

$$\frac{dx}{dt} = u + a \quad (39)$$

$$\frac{\delta P}{\delta t_+} + \frac{a}{c_p} \frac{\delta S}{\delta t_+} + (\alpha - 1) \frac{au}{r} = 0 \quad (40)$$

and along a left running characteristic or Q-wave,

$$\frac{dx}{dt} = u - a \quad (41)$$

$$\frac{\delta Q}{\delta t_-} + \frac{a}{c_p} \frac{\delta S}{\delta t_-} + (\alpha - 1) \frac{au}{r} = 0 \quad (42)$$

In the present explosion case, a Q-rarefaction wave results. The values of Q in the plane case for state (4) and (3) are  $2a_4/(\gamma_4 - 1)$  and  $2a_3/(\gamma_4 - 1) - u_3$ , respectively. In the limit for a complete rarefaction wave when  $a_3 \rightarrow 0$ ,  $u_3 \rightarrow 2a_4/(\gamma_4 - 1)$  and  $Q \rightarrow -2a_4/(\gamma_4 - 1)$ . Consequently, Q decreases from the head  $[Q = 2a_4/(\gamma_4 - 1)]$  to the tail of the rarefaction wave. Since the Q-rarefaction wave is isentropic, Eq. (42) gives  $\delta Q/\delta t_- = -(\alpha - 1)au/r$ , that is, as one proceeds along a Q characteristic Q decrease. This can only happen if the characteristic accelerates in the direction of the tail of the rarefaction wave. In other words, as time goes on, the Q-rarefaction wave continues to get stronger until it is engulfed by the second shock wave.

The pressure profiles obtained by Sod's method are displayed in Fig. 12. The numerical results are drawn from the output of the computer without smoothing (except in Fig. 15, the explosion-wave diagram). The results exhibit the general characteristics of a Q-rarefaction wave for an explosion problem very well. Initially the planar rarefaction strength  $p_{01} = 0.356$ . As time goes on, the absolute values of pressures at the tail of the rarefaction wave continue to decrease until the second shock wave is generated around the time number 10 which corresponds to  $26.5 \mu s$  after the glass sphere ruptures. At time number 10, the rarefaction strength is increased to 0.142. The density profiles are shown in Fig. 13. They are quite similar to the pressure profiles except for the discontinuity across the contact surface. Again, the lowered density ratios or increased rarefaction-wave strengths are observed. The formation of a second shock wave and the deceleration of the primary shock wave can be explained by considering the path of the contact surface as similar to that of a piston. The contact surface is decelerated as a result of the spherical nature of the flow and sends out ahead of itself rarefaction pulses (P-characteristics) that overtake and decay the primary shock wave. However, behind it, compression pulses (Q-characteristics) are sent out which overtake to form a second shock (implosion) wave along the tail of the rarefaction wave. (It is worth noting that in the planar case such pulses run parallel to the tail of the wave, but in cylindrical and spherical flows, they collide with the tail of the rarefaction wave.) This explains why the path of second shock is connected with the tail of the rarefaction wave. Although the second shock wave is a backward facing wave, it is initially very weak and propagates outward at first owing to the high positive particle velocity. However, as it gains strength, it overcomes this counter flow and finally implodes on the origin with unlimited strength ideally. In Figs. 12-a and 13, we can see that the strength of the primary shock wave decays as it proceeds and how the second shock wave is generated. In the foregoing figures at about  $26.5 \mu s$  after rupture (time number 10), noticeable discontinuities were found that grew into a second shock wave, and were defined as the birth point of the second shock wave. The particle-velocity profiles are shown in Fig. 14. In the early stage of the explosion, all particles move outward (positive velocity). As the contact surface decelerates, compression waves (Q-characteristics) and rarefaction waves (P-characteristics) decelerate the particle velocity creating a large negative velocity range. In this particular case, it reaches almost  $-0.8a_1$  (at time number 46,  $120 \mu s$  after rupture). This negative particle velocity is reversed by the reflected second shock up to small positive values (time number 56). In Figs. 12, 13 and 14, the profiles of  $\rho$ ,  $p$  and  $u$  have complex structures around the origin. This is mainly due to the randomness of the RCM in the rarefaction wave. Unlike similarly-facing shock waves in the planar case, the second shock wave does not overtake the primary shock wave because of the lower sound speed and the lower or even opposing particle velocity behind the primary shock wave. Therefore, the primary shock wave and the reflected second shock wave slow down continuously to become Mach waves. (It is worth noting that this is the principle behind travelling wave sonic-boom simulators; Ref. 33.)

The wave diagram is shown in Fig. 15. Isobars, isopycnics and isotachs (constant velocity lines) are shown in Figs. 16, 17 and 18, respectively. In the figures, the decreases in pressure and density behind the incident and reflected rarefaction waves are quite apparent. The pressures and densities in front of the imploding shock wave near the origin are very small. This imploding shock wave also induces large negative velocities as it approaches the origin and a line of zero particle velocity is seen. It is also apparent that the second shock wave is

produced along the tail of the rarefaction wave, propagates outward at first, then starts to implode and increases in strength to unlimited values as it hits the origin and reflects. The origin becomes a singularity and the continuum equations break-down. Transport properties would keep the thermodynamic properties finite at the implosion focus.

## 4.2 REACTING-GAS FLOW

### 4.2.1 GENERAL DESCRIPTION

The RCM was applied to reacting gas flow by Chorin (Ref. 7) and was shown to be capable of handling time-dependent detonation and deflagration waves with finite and infinite reaction rate. Chorin emphasized an important advantage of using his method since the interaction of the flow and the chemical reaction can be taken into account when the Riemann problem is solved, even when the time scales of the chemistry and the fluid flow are very different. As a result, the basic conservation laws are satisfied at the end of each time step. If the chemical reactions and the gas flow were to be taken into account in separate fractional steps, the basic conservation laws may be violated at the end of each hydrodynamic step, thus either inducing unwanted oscillations and waves, or requiring time steps small enough for all changes to be very gradual, usually a costly remedy. Chorin's main object seemed to be placed on developing the technique and to show the usefulness of the method. Thus, in his program, there is an unreasonable assumption,  $\gamma_0 = \gamma_1 = \gamma$ , i.e., the specific heat ratios do not change across the reaction front. Although, as he states in his paper, the case  $\gamma_0 \neq \gamma_1$  is more difficult only because of additional algebra. We felt that this assumption must be improved. Here, as a first step, the program was modified to have changes in the specific heat ratio so that  $\gamma_0 \neq \gamma_1$  at the detonation-wave front. The RCM was then applied to a detonation wave in a  $2H_2 + O_2$  gas mixture.

### 4.2.2 CHAPMAN-JOUQUET DETONATION

A Chapman-Jouquet detonation is described briefly in this section for the convenience of explaining Chorin's method of calculating reacting-gas flow. The equations to be solved are (Ref. 7 and 34)

$$\rho_t + (\rho u)_x = 0 \quad (43)$$

$$(\rho u)_t + (\rho u^2 + p)_x = 0 \quad (44)$$

$$e_t + [(e + p)u]_x = 0 \quad (45)$$

where

$$e = \rho \epsilon + \frac{1}{2} \rho u^2 \quad (46)$$

$$\epsilon = \epsilon_1 + q \quad (47)$$

$\epsilon_1$  is the internal energy per unit mass and expressed as,

$$\epsilon_1 = \frac{1}{\gamma - 1} \frac{p}{\rho} \quad (48)$$

$q$  is the energy of formation which can be released through chemical reaction. In this present section, it is assumed that part of  $q$  is released instantaneously in an infinitely thin reaction zone. Denoting the unburned and the burned gas with 0 and 1, respectively, we have

$$\epsilon_0 = \frac{1}{\gamma_0 - 1} \frac{p_0}{\rho_0} + q_0 \quad (49)$$

$$\epsilon_1 = \frac{1}{\gamma_1 - 1} \frac{p_1}{\rho_1} + q_1 \quad (50)$$

Assuming that the unburned gas is on the right, and letting  $D$  be the velocity of the reacting zone, Eqs. (43) and (44) can be written in conservation form

$$\rho_1 w_1 = \rho_0 w_0 = -M \quad (51)$$

$$\rho_0 w_0^2 + p_0 = \rho_1 w_1^2 + p_1 \quad (52)$$

where

$$w_0 = u_0 - D, \quad w_1 = u_1 - D \quad (53)$$

From these relations one readily deduces

$$M^2 = -(p_0 - p_1)/(\tau_0 - \tau) \quad (54)$$

where  $\tau$  is the specific volume,  $1/\rho$ .

Conservation of energy is expressed by

$$\epsilon_1 - \epsilon_0 - \frac{1}{2} (\tau_0 - \tau_1)(p_0 + p_1) = 0 \quad (55)$$

Substituting Eqs. (49) and (50) into Eq. (55), we have

$$\left( p_0 + \frac{\gamma_1 + 1}{\gamma_0 - 1} p_1 \right) \tau_1 - \left( p_1 + \frac{\gamma_1 + 1}{\gamma_0 - 1} p_0 \right) \tau_0 + 2\Delta = 0 \quad (56)$$

where  $\Delta \leq q_1 - q_0$ . In the  $(\tau_1, p_1)$ -plane the lines through  $(\tau_0, p_0)$  tangent to the curve expressed by Eq. (56) are called the Rayleigh lines (Fig. 19). Their points of tangency,  $S_1$  and  $S_2$  are called the Chapman-Jouguet (CJ) points. The upper portion of the curve corresponds to detonations; the portion above  $S_1$

to strong detonations and the portion below to weak detonations. The lower part of the curve corresponds to deflagrations. A portion of the curve is omitted as it corresponds to physically unacceptable conditions where  $M^2 < 0$ . The velocity and strength of a strong detonation are entirely determined by the state of the unburned gas in front of the detonation and one quantity behind the detonation just as for shock waves. Let  $p_0$ ,  $\rho_0$  and  $u_0$  be given, as well as  $p_1$ , and assume the unburned gas lies to the right of the detonation, then from Eq. (56)

$$\tau_1 = \tau_0 \left( \frac{\mu_1^2}{\mu_0^2} p_0 + \mu_1^2 p_1 \right) / (\mu_1^2 p_0 + p_1) - 2\mu_1^2 \Delta / (\mu_1^2 p_0 + p_1) \quad (57)$$

where

$$\mu_i^2 = \frac{\gamma_i - 1}{\gamma_i + 1}, \quad i = 0, 1 \quad (58)$$

and

$$M^2 = \rho_0(p_0 - p_1)(\mu_1^2 p_0 + p_1) / \left\{ \left( \frac{\mu_1^2}{\mu_0^2} - \mu_1^2 \right) p_0 + (\mu_1^2 - 1)p_1 - 2\mu_1^2 \rho_0 \Delta \right\} \quad (59)$$

The states on the curve located between the CJ point  $S_1$  and the line  $\tau = \tau_0$  correspond to weak detonations. In this region, a CJ-detonation is followed by a rarefaction wave.

In what follows an explicit criterion for determining whether a detonation will be a strong detonation or a CJ-detonation is described. It is shown in Ref. 34 that at  $S_1$ , the velocity  $|w_1| = a_1$  where  $a_1 = (\gamma_1 p_1 / \rho_1)^{1/2}$  is the sound speed, i.e., a CJ-detonation moves with respect to the burned gas with a velocity equal to the velocity of sound in the burned gas. This fact is used to determine the density  $\rho_{CJ}$ , velocity  $u_{CJ}$ , and pressure  $p_{CJ}$  behind a CJ-detonation. From Eqs. (51) and (54)

$$(p_1 - p_0) / (\tau_1 - \tau_0) = -\rho_1^2 w_1^2 = -\rho_1^2 \frac{\gamma_1 p_1}{\rho_1} \quad (60)$$

Therefore we get

$$\tau_1 = \gamma_1 \tau_0 p_1 / \{(\gamma_1 + 1)p_1 + p_0\} \quad (61)$$

From Eqs. (56) and (61) we have,

$$p_1^2 + 2bp_1 + c = 0 \quad (62)$$

where

$$b = - \frac{\gamma_1 - 1}{\gamma_0 - 1} p_0 + (\gamma_1 - 1) \rho_0 \Delta \quad (63)$$

$$c = \frac{\mu_1^2}{\mu_0} p_0 - 2\mu_1^2 \rho_0 p_0 \Delta \quad (64)$$

Therefore

$$p_{CJ} = p_1 = -b + (b^2 - c)^{1/2} \quad (65)$$

Given  $p_{CJ}$ ,  $\rho_{CJ} = \rho_1 = \tau_1^{-1}$  can be obtained from Eq. (61). Since  $M = -\rho_1 w_1$  and  $w_1 = -a_1$ , we find

$$M = (\gamma_1 p_1 \rho_1)^{1/2} = (\gamma_1 p_{CJ} \rho_{CJ})^{1/2}$$

The velocity of the CJ-detonation wave  $D_{CJ}$  is found from

$$\rho_0 (u_0 - D_{CJ}) = -M$$

which yields  $D_{CJ} = \{\rho_0 u_0 + (\gamma_1 p_{CJ} \rho_{CJ})^{1/2}\} / \rho_0$  and then

$$u_{CJ} = D_{CJ} - a_{CJ}$$

Suppose  $u_1$ , the velocity of the burned gas, is given. If  $u_1 < u_{CJ}$  a CJ-detonation appears, followed by a rarefaction wave. If  $u_1 = u_{CJ}$  a CJ-detonation appears alone, and if  $u_1 > u_{CJ}$  a strong detonation takes place.

An outline of Chorin's method for calculating reacting-gas flows is described in the next section.

#### 4.2.3 CHORIN'S METHOD FOR REACTING-GAS FLOWS

In this section, Eq. (47) is replaced by

$$\epsilon = \frac{1}{\gamma - 1} \frac{p}{\rho} + Zq \quad (66)$$

where  $Z$  is a progress parameter for the reaction, and  $q$  is the total available binding energy ( $q \leq 0$ ).  $Z$  is assumed to satisfy the rate equation,

$$dZ/dt = -KZ \quad (67)$$



where

$$K = 0 \quad \text{if} \quad T = \frac{p}{\rho} \leq T_0$$

$$K = K_0 \quad \text{if} \quad T = \frac{p}{\rho} > T_0$$
(68)

$T_0$  is the ignition temperature and  $K_0$  is the reaction rate. Chorin has solved Eqs. (43), (44), (45), (46), (66), (67) and (68) using the RCM and has shown that a Riemann type problem can be solved even when deflagrations and detonations are included along with shock and rarefaction waves. In the present case, the initial data for a Riemann problem has the form of

$$\left. \begin{aligned} S_l(\rho = \rho_l, p = p_l, u = u_l, Z = Z_l) \text{ for } x \leq 0 \\ \text{and} \\ S_r(\rho = \rho_r, p = p_r, u = u_r, Z = Z_r) \text{ for } x > 0 \end{aligned} \right\} \quad (69)$$

When there is no chemistry ( $K_0 = 0$ ),  $Z = \text{constant}$  and Eq. (69) reduces to Eq. (7) and its solution is given in Chapter 2. In case  $K_0 \neq 0$ , right and left waves may now be CJ or strong-detonation waves as well as shock and rarefaction waves. Chorin has incorporated these possibilities into the solution of the Riemann problem and developed a computer program to calculate this problem.

The state  $S_r$  remains a constant state;  $u_r$  and  $p_r$  are fixed. The energy in  $S_r$  must change at constant volume (and thus can do no work). The change  $\delta Z_r$  in  $Z_r$  can be found by integrating Eqs. (67) and (68), with  $Z(0) = Z_r$  and  $Z(\Delta t/2) = Z_r + \delta Z_r$ ,  $\delta Z_r < 0$ . The new pressure is written as

$$p_r^{\text{new}} = p_r + \delta p_r = p_r + (\gamma - 1) Z \delta \rho_r \quad (70)$$

In what follows, the superscript new, is dropped. Similarly,  $Z_l$  changes to  $Z_l + \delta Z_l$ , and a new  $p_l$  is found using the analog of Eq. (70).

In  $S_*$  the values of  $Z$  differ from the values  $Z_r + \delta Z_r$ ,  $Z_l + \delta Z_l$ . Let  $Z_{*l}$  be the value of  $Z$  to the left of the slip line ( $dx/dt = u_*$ ) and let  $Z_{*r}$  be the value of  $Z$  to the right of the slip line. The difference in energy of formation across the right wave is  $\Delta_r = [Z_{*r} - (Z_r + \delta Z_r)]q$ , and across the left wave it is  $\Delta_l = [Z_{*l} - (Z_l + \delta Z_l)]q$ . Iteration will be carried out on the values  $Z_{*l}$ ,  $Z_{*r}$ ,  $\Delta_l$ ,  $\Delta_r$ . In the first iteration, Eqs. (19) to (22) are iterated with  $Z_{*r} = Z_r + \delta Z_r$ ,  $Z_{*l} = Z_l + \delta Z_l$ , and thus  $\Delta_l = \Delta_r = 0$ . When this iteration has converged, a new pressure  $p_*$  is given, and new densities  $\rho_{*l}$ ,  $\rho_{*r}$  can be found from Eqs. (9), (16) or the isentropic equation of state. New temperatures  $T_{*l} = p_*/\rho_{*l}$ ,  $T_{*r} = p_*/\rho_{*r}$ , are evaluated, Eqs. (67) and (68) are solved, and new values  $Z_{*l}$ ,  $Z_{*r}$ ,  $\Delta_l$ ,  $\Delta_r$  are found. If  $\Delta_r > 0$  the right wave is either a shock or a rarefaction wave, and if  $\Delta_r < 0$  the right wave is either a CJ-detonation followed by a rarefaction wave or a strong detonation.

Let  $u_*$  be the velocity in  $S_*$ . Given  $\Delta_l$ ,  $\Delta_r$ , we can find the velocities  $u_{CJl}$ ,  $u_{CJr}$  behind possible CJ-detonations on the right and left. If  $u_* \leq u_{CJr}$

the right wave is a CJ-detonation followed by rarefaction, and if  $u_* \geq u_{CJ_r}$  the right wave is a strong detonation. The CJ state is unaffected by  $S_*$  (since it depends only on  $S_r$ ) and as far as the Riemann solution is concerned it is a fixed state. If the right wave is a CJ-detonation,  $M_r$  is redefined as

$$M_r = (p_{CJ} - p_*) / (u_{CJ} - u_*)$$

where  $p_{CJ}$  is from Eq. (65) and then

$$M_r = (\rho_{CJ} p_{CJ})^{1/2} \phi_2(p_*/p_{CJ}), \quad p_*/p_{CJ} \leq 1 \quad (71)$$

$\phi_2$  is defined in Eq. (13). If the right wave is a strong detonation, from Eq. (59),

$$M_r = \rho_r^{1/2} \phi_3(\rho_r \Delta_r, p_r, p_*)$$

where

$$(\phi_3)^2 = \frac{(p_r - p_*)(\mu_1^2 p_r + p_*)}{\left(\frac{\mu_1^2}{\mu_0^2} - \mu_1^2\right) p_r + (\mu_1^2 - 1)p_* - 2\mu_1^2 \rho_r \Delta_r} \quad (72)$$

Similar expressions occur on the left. A second iteration starts with  $M_\ell$ ,  $M_r$  from the previous iteration, and written out in full, appears as follows:

$$p_*^v = (u_\ell - u_r + p_r/M_r^v + p_\ell/M_\ell^v) / (1/M_\ell^v + 1/M_r^v) \quad v \geq 0$$

$$p_*^{v+1} = \max(\epsilon, p_*^v)$$

$$u_*^v = (p_\ell - p_r + M_\ell^v u_\ell + M_r^v u_r) / (M_\ell^v + M_r^v)$$

where

$$(\rho_r, p_r, u_r) = (\rho_{CJ_r}, p_{CJ_r}, u_{CJ_r}) \quad \text{if right wave = CJ-detonation,}$$

$$= (\rho_r, p_r, u_r) \quad \text{otherwise,}$$

$$(\rho_\ell, p_\ell, u_\ell) = (\rho_{CJ_\ell}, p_{CJ_\ell}, u_{CJ_\ell}) \quad \text{if left wave = CJ-detonation,}$$

$$= (\rho_\ell, p_\ell, u_\ell) \quad \text{otherwise,}$$

$$M_r^{v+1} = \rho_r^{1/2} \phi_3(\rho_r \Delta_r, p_r, p_*^{v+1}) \quad \text{if right wave = strong detonation,}$$

$$= (\rho_r p_r)^{1/2} \phi(p_*^{v+1}/p_r) \quad \text{otherwise}$$

$$M_l^{v+1} = \rho_l^{1/2} \phi_3(\rho_l \Delta_l, p_l, p_*^{v+1}) \quad \text{if left wave = strong detonation,}$$

$$= (\rho_l p_l)^{1/2} \phi(p_*^{v+1}/p_l) \quad \text{otherwise.}$$

The iteration is stopped when it has converged, as before. New values of  $Z_{*l}$ ,  $Z_{*r}$ ,  $\Delta_l$ ,  $\Delta_r$  are evaluated, and the iteration is repeated. This process is stopped when  $\Delta_l$ ,  $\Delta_r$  change by less than some predetermined  $\epsilon_3$  over two successive iterations. Once  $S_x$  has been determined, the solution is sampled as described in Chapter 2. The only difference in the sampling procedure is that, if the wave is CJ-detonation,  $(\rho_r, p_r, u_r)$  are replaced by  $(\rho_{CJr}, p_{CJr}, u_{CJr})$  in all equations which describe the flow to the left of the detonation wave. Similarly  $(\rho_l, p_l, u_l)$  are replaced by  $(\rho_{CJl}, p_{CJl}, u_{CJl})$  if the left wave is CJ-detonation wave. More details can be found in Ref. 7.

#### 4.2.4 NUMERICAL RESULTS

In Ref. 7, Chorin has displayed numerical results in cases of a strong detonation wave, a CJ-detonation wave and a deflagration wave. However, those examples were meant to show the usefulness of the method while using only a small number of mesh points. Besides, the assumption  $\gamma_0 = \gamma_1$  is quite a rough assumption from the point of view of actual applications. Here a practical case has been calculated in which the burned gas has different specific heat ratio from the unburned gas. It is assumed that a combustible gas mixture reacts in an infinitely thin reaction zone and turns into reaction products instantaneously and its composition stays the same afterward, namely, the specific heat ratio and the specific molecular weight change their values at the wave front from  $\gamma_0$  to  $\gamma_1$  and  $M_0$  to  $M_1$ , respectively. A stoichiometric gas mixture of hydrogen and oxygen was chosen as an example. The data on combustion products were taken from the results obtained by Benoit (Refs. 35 and 36). Those conditions are:

unburned gas:  $2H_2 + O_2$  gas mixture  
 $\gamma_0 = 1.40$ ,  $M_0 = 12.0$

reaction products:  $H_2O$  (53.2%),  $OH$  (13.7%),  $H_2$  (16.4%)  
 $O_2$  (4.9%),  $H$  (8.1%),  $O$  (3.8%)  
 $\gamma_1 = 1.22$ ,  $M_1 = 14.5$

From these values, the released energy was calculated to be 22.95 K cal/mol. Under these assumptions and conditions, a CJ-detonation resulted, followed by a rarefaction wave. The pressure profiles are shown in Fig. 20. Although it takes some time for the CJ-detonation to be fully developed, the pressure profiles are quite similar once CJ-detonation is established. At the wave front, the pressure ratio  $p/p_0$  jumps from 1 to a value of about 15 for a CJ-detonation. It then decays to a fairly constant stationary state in which  $p/p_0$  is about 6, due to the rarefaction wave. This stationary state seems to extend from the starting position of the detonation wave to about half of the distance which the detonation

wave has travelled in the channel.

The pressure profiles of the reflected detonation wave as a shock wave at the end wall of the combustion tube is shown in Fig. 21. Since the reflected shock wave is propagating in a non-uniform state, the profiles of the reflected shock wave change accordingly. At the moment, when the detonation wave reflects at the end wall, the pressure ratio  $p/p_0$  is as high as 25 (this may be compared with the highest value of 8 for an intense planar shock wave). Later, when the reflected shock wave is propagating in the fairly uniform region  $p/p_0$  is about 12. In the sense that the data for the reaction products are needed as inputs for the computation, the program can still be improved. If a program which calculates the chemical reactions and determines the reaction products will be combined with Chorin's method, it will form a very important, useful and generalized method of calculating reacting-gas flows.

## 5. DISCUSSIONS AND CONCLUSIONS

It has been shown by using an extensive number of examples that the RCM provides exceptionally high computational accuracy for flows involving planar and spherical shock waves, rarefaction waves and contact surfaces, as well as their interactions. In addition, the RCM can handle flows with detonations and chemical reactions involving the above transition fronts.

Owing to the high accuracy of calculated values in  $p$ ,  $\rho$ ,  $u$  and the fact that the constant states are perfectly realized, very complex wave-interaction problems which involve small changes in physical parameters  $\rho$ ,  $u$ ,  $p$ , can be calculated, such as the reflection of a shock wave from the end wall of a shock tube and the subsequent interactions, or the head-on collision of a shock wave with a rarefaction wave.

Although, in practice, the accuracy of the wave positions is good (1 ~ 3% of the total length of the spatial zones in the examples investigated here), Glimm has recently developed "the method of tracking discontinuities", which improves this spatial error by a factor of 4 to 10 and locates the transition fronts with an accuracy of  $0.05\Delta x$  to  $0.5\Delta x$  (Ref. 37). This improvement must be greatly appreciated when one tries to apply the RCM to multidimensional wave-interaction problems where the number of mesh points used and the computation time are competitive.

Due to the randomness of the method, the rarefaction waves are not smooth. However, Sod states in his paper (Ref. 4) that the rarefaction wave obtained by the RCM could be smoothed out by a type of averaging and that he was considering this subject. Once this has been accomplished, it is expected that the RCM will increase its usefulness and applicability to those wave-interaction problems in which rarefaction waves are involved in a more complex manner.

There are a number of very important pseudo-stationary problems, such as oblique-shock-wave reflections (Ref. 1), which require new approaches to their numerical solutions. It is possible that the RCM may be ideally suited to the solution of regular, single-Mach, complex-Mach and double-Mach-reflection problems of oblique shock waves. A start in their direction has already been made for stationary regular and Mach oblique-shock-wave reflection by Chorin (Ref. 3). We are hopeful that complex-Mach and double-Mach reflections will be solved in the same manner and perhaps extended to similar reflections of spherical shock waves.

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## APPENDIX A: CONTACT SURFACE MOTION

When wave interactions are considered in a flow field which involves different gases with different specific heat ratios, it is necessary to know the positions of the contact surfaces, across which the specific heat ratios change their values. The method used here for determining the paths of contact surfaces is as follows.

In principle, as previously mentioned, solutions  $\bar{p}$ ,  $\bar{u}$ ,  $\bar{p}$  are determined at points  $(i\Delta x, n\Delta t)$  and  $\{(i + 1/2)\Delta x, (n + 1/2)\Delta t\}$ . In a real program, however, the calculation is carried out in a two-step method and there are no intermediate spatial mesh points like  $(i + 1/2)\Delta x$ . At the end of the first half-step, those solutions which are supposed to be placed at points  $\{(i + 1/2)\Delta x, (n + 1/2)\Delta t\}$  will be stored in mesh points  $\{(i + 1)\Delta x, (n + 1/2)\Delta t\}$ ; namely, storing positions are shifted at half-mesh intervals,  $1/2 \Delta x$ , to the right. On the other hand, at the end of the second half-step, solutions are stored after being shifted  $1/2 \Delta x$  to the left. Figure A-1 illustrates this procedure. We can see that at the end of every other half time-step, the mesh points correspond to the same physical positions. Considering this procedure, we can determine the position of contact surfaces and assign the different values of the specific heat ratio  $\gamma$ . Suppose a contact surface was located between the  $i$ -th mesh and the  $(i-1)$ -th mesh at the beginning of the first half-step, i.e.,

$$\left. \begin{array}{l} \gamma(i) = \gamma_1 \\ \gamma(i-1) = \gamma_2 \end{array} \right\} \text{ at } t = n\Delta t$$

and one of the regions to the left of the contact surface was chosen by sampling. Then, as described before, the solution which is associated with this region will be given to the  $i$ -th mesh point. This means that the contact surface has moved one mesh to the right, namely, from the mesh  $(i-1)$  to the mesh  $i$ . When sampling point  $P$  lies to the right of the contact surface, the solution associated with one of the regions having the specific heat ratio  $\gamma_1$  will be assigned to the mesh  $i$ . This situation corresponds to a situation where the contact surface did not move at all because the distribution of  $\gamma$  is the same as before. In the second half-step, the movement of a contact surface is determined in the same manner as in the first half-step, except that, in this case, the movement of a contact surface is either one mesh to the left or stays in the same position. Figure A-2 and Table A-1 illustrate the propagation of a contact surface.



## APPENDIX B: PROGRAM LISTINGS

In the program, all dependent thermodynamic and dynamic values are made nondimensional as follows

$$\bar{p} = \frac{p}{p_1}, \quad \bar{\rho} = \frac{\rho}{\rho_1}, \quad \bar{u} = \frac{\sqrt{\gamma_1} u}{a_1}$$

The independent variables of time and distance are also made nondimensional so that

$$\bar{t} = \frac{a_1 t}{\sqrt{\gamma_1} L} \quad \text{and} \quad \bar{x} = \frac{x}{L}$$

where  $L$  is the total length of a shock tube or the radius of an initial cylindrical or spherical charge. The program consists of one main program and five subroutines. Their functions will be described briefly.

Initial conditions; type of flow such as plane, cylindrical or spherical; how and how often the output should be printed; mesh number; when to stop the calculation; the boundary conditions are put into the main program. The main program determines the time increment  $DT(\Delta t)$ , and spatial increment  $DX(\Delta x)$ , in such a way that the Courant condition is satisfied, though the method itself is stable, even if the Courant condition is violated. A random number  $XI(\theta_n)$ , is determined at each half-time step with the aid of the SUBROUTINE RANDU which is designed by IBM to generate random number, YFL over (0, 1). Then, at each mesh point, the Riemann problem is solved calling the SUBROUTINE GLIMM. It solves the Riemann problem receiving the two initial state  $S_l$  and  $S_r$  from the main program and does the sampling according to the random number  $XI$ . In the course of solving the Riemann problem, FUNCTION FAI which corresponds to the function  $\phi$  in Eqs. (11), (13) and (17) in Chapter 2 is used. By putting the sampled solutions into each mesh, the first half-step is finished. Repeating the same procedure for the second half-step, one time step is finished and the solutions for a planar waves are obtained. Boundary conditions are taken into consideration when  $S_l$  and  $S_r$  are chosen in the main program. The results are printed calling the SUBROUTINE STTOUT. If either a cylindrical or spherical flow is needed to be solved, Eq. (36) in Sec. 4.1.2 is solved after the planar case has been solved. This is done calling SUBROUTINE INHOM.

# LISTING OF THE COMPUTER PROGRAM

```

C          RANDOM CHOICE METHOD   VARIATION 2.
C          PROGRAM FOR EXPLOSION OF A PRESSURIZED HELIUM SPHERE
1  COMMON/DT,RL,UL,PL,R,U,P,E,RR,UR,PR,XI,Y,GAMMAL,GAMMAR
2  COMMON/OUT/TIME,N,DX,RHO(301),PRE(301),UX(301),ENG(301),GAMMA(301)
3  COMMON/RAD/ETA
4  INTEGER TSTP
5  NSTOP=320
6  NPRINT=5
7  N=180
8  NP1=N+1
9  NHALF=34
10 NHALP1=NHALF+1
11 DX=1./FLOAT(N)
12 DT=0.01
13 TIME=0.
14 VMAX=0.
15 NCNTCT=NHALP1
16 NINCRS=0
17 GAMMRI=1.400
18 GAMMLI=1.667
19 K1=11
20 K2=7
21 NU=2
22 SIGMA=.5
23 ETA=3.
C          SFT INITIAL CONDITIONS
24 DO 83 I=1,NP1
25   IF(I.GE.NCNTCT) GO TO 11
26   GAMMA(I)=GAMMLI
27   GO TO 83
28 11 GAMMA(I)=GAMMRI
29 83 CONTINUE
30   PL=18.25
31   RL=2.523
32   UL=0.
33   PR=1.
34   RR=1.
35   UR=0.
36   DO 15 I=1,NHALF
37    RHO(I)=RL
38    PRE(I)=PL
39    UX(I)=UL
40 15 CONTINUE
41   DO 16 I=NHALP1,NP1
42    RHO(I)=RR
43    PRE(I)=PR
44    UX(I)=UR
45 16 CONTINUE
C          BEGIN TIME STEP
46   IX=123456789
47   DO 100 TSTP=1,NSTOP
48   DO 8 I=2,N
49   VMAX1=ABS(UX(I))+SQRT(GAMMA(I)*PRE(I)/RHO(I))

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50      IF(VMAX1 .GT. VMAX) VMAX=VMAX1
51      B CONTINUE
52      DTT=SIGMA*DX/VMAX
53      IF(DTT .LT. DT) DT=DTT
54      TIME=TIME+2.*DT
      C COMPUTE FIRST HALF STEP
      C GENERATE RANDOM SI USING CHORIN'S METHOD
55      NU=MOD(NU+K2,K1)
56      CALL RANDU(IX,IY,YFL)
57      SI=(YFL+FLOAT(NU))/FLOAT(K1)
      C XI LIES BETWEEN -DX/2 AND DX/2
58      XI=SI*DX-0.5*DX
59      DO 40 I=2,NP1
60      RR=RHO(I)
61      UR=UX(I)
62      PR=PRE(I)
63      GAMMAL=GAMMA(I-1)
64      GAMMAR=GAMMA(I)
65      IF(I .EQ. 2.) GO TO 43
66      RL=RIM1
67      PL=PIM1
68      UL=UIM1
69      GO TO 44
      C BOUNDARY CONDITION AT AXIS R=0.
70      43 RL=RR
71      UL=-UR
72      PL=PR
      C COMPUTE FIRST HALF STEP OF GLIMM
73      44 CALL GLIMM
74      IF(I.NE.NCNTCT) GO TO 35
75      NINCRS=1
76      IF(XI.GE.Y) NINCRS=0
77      35 RIM1=RHO(I)
78      RHO(I)=R
79      PIM1=PRE(I)
80      PRE(I)=P
81      UIM1=UX(I)
82      UX(I)=U
83      40 CONTINUE
84      NCNTCT=NCNTCT+NINCRS
85      DO 75 I=1,NP1
86      IF(I.GE.NCNTCT) GO TO 4
87      GAMMA(I)=GAMMLI
88      GO TO 75
89      4 GAMMA(I)=GAMMRI
90      75 CONTINUE
      C COMPUTE SECOND HALF STEP
      C GENERATE RANDOM SI USING CHORIN'S METHOD
91      NU=MOD(NU+K2,K1)
92      CALL RANDU(IX,IY,YFL)
93      SI=(YFL+FLOAT(NU))/FLOAT(K1)
      C XI LIES BETWEEN -DX/2 AND DX/2
94      XI=SI*DX-0.5*DX
95      DO 60 I=1,N
96      RL=RHO(I)
97      PL=PRE(I)
98      UL=UX(I)
99      GAMMAL=GAMMA(I)
100     GAMMAR=GAMMA(I+1)
101     IF(I .EQ. N) GO TO 63

```

```

102      RR=RHO(I+1)
103      PR=PRE(I+1)
104      UR=UX(I+1)
105      GO TO 64
      C   HOUNDARY CONDITION AT R=1.
106      63 RR=RL
107      UR=-UL
108      PR=PL
      C   COMPUTE SECOND HALF STEP OF GLIMM
109      64 CALL GLIMM
110      NCNTM1=NCNTCT-1
111      IF(I.NE.NCNTM1) GO TO 55
112      NINCRS=-1
113      IF(X1.LT.Y) NINCRS=0
114      55 RHO(I)=R
115      PRE(I)=P
116      UX(I)=U
117      60 CONTINUE
118      NCNTCT=NCNTCT+NINCRS
119      DO 70 I=1,NP1
120      IF(I.GE.NCNTCT) GO TO 3
121      GAMMA(I)=GAMMLI
122      GO TO 70
123      3 GAMMA(I)=GAMMRI
124      70 CONTINUE
125      CALL INHOM
126      IF(MOD(TSTP,NPRINT).EQ.0) CALL STTOUT
127      100 CONTINUE
128      STOP
129      END

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130      SUBROUTINE GLIMM
131      COMMON//DT,RL,UL,PL,R,U,P,E,RR,UR,PR,XI,Y,GAMMAL,GAMMAR
132      REAL MR,ML,MRP1,MLP1
133      EPS=1.0E-6
134      IT=0
135      ITSTOP=20
      C      CONSTRUCTION OF RIEMANN PROBLEM
      C      ALFA IS THE CONVERGENCE FACTOR
      C      INITIAL ML AND MR
136      ALFA=1.
137      ALFAM=1.-ALFA
138      ML=100.
139      MR=100.
140      COEFL=SQRT(PL*RL)
141      COEFR=SQRT(PR*RR)
142      PSTAR=.5*(PL+PR)
      C      SOLVE RIEMANN PROBLEM USING GODUNOV'S ITERATIVE METHOD
143      10 IT=IT+1
      C      IF PSTAR IS LESS THAN EPS THEN PSTAR IS SET EQUAL
      C      TO 1.0E-6 TO PREVENT PSTAR FROM BECOMING NEGATIVE.
144      IF(PSTAR.LT.EPS) PSTAR=EPS
      C      COMPUTE MR AND ML AT STEP Q+1
145      MLP1=COEFL*PHI(PSTAR/PL,GAMMAL)
146      MRP1=COEFR*PHI(PSTAR/PR,GAMMAR)
147      DIFML=ABS(MLP1-ML)
148      DIFMR=ABS(MRP1-MR)
149      ML=MLP1
150      MR=MRP1
      C      COMPUTE NEW PRESSURE PSTAR
151      PSTARP=PSTAR
152      PSTAR=(UL-UR+PR/MR+PL/ML)/(1./ML+1./MR)
153      PSTAR=ALFA*PSTAR+ALFAM*PSTARP
154      IF(IT .LE. ITSTOP) GO TO 30
155      IF(ABS(PSTAR-PSTARP) .LT. EPS) GO TO 40
156      IF(DIFML*DIFMR .LT. EPS) GO TO 40
157      ALFA=ALFA/2.
158      ALFAM=1.-ALFA
159      IF(ALFAM .LT. EPS) GO TO 40
160      IT=0
161      30 IF(DIFML .GT. EPS) GO TO 10
162      IF(DIFMR .GT. EPS) GO TO 10
      C      COMPUTE USTAR AT END OF GODUNOV ITERATION
163      40 USTAR=(PL-PR+MR*UR+ML*UL)/(ML+MR)
      C      BEGIN GLIMM'S METHOD
164      IREGL=1
165      IF(PSTAR .LT. PL) IREGL=2
166      IREGR=1
167      IF(PSTAR .LT. PR) IREGR=2
168      X=USTAR*DT
169      Y=X

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170      IF(XI .GE. X) GO TO 200
      C      LEFT SIDE
171      IF(IREGL .EQ. 2) GO TO 110
      C      COMPUTE LEFT SHOCK SPEED
172      U=UL-ML/RL
173      X=U*DT
174      IF(XI .GE. X) GO TO 100
      C      LEFT OF LEFT SHOCK
175      R=RL
176      U=UL
177      P=PL
178      GO TO 500
      C      RIGHT OF LEFT SHOCK
179      100 R=ML/(USTAR-U)
180      U=USTAR
181      P=PSTAR
182      GO TO 500
      C      COMPUTE SOUND SPEED IN LEFT STATE
183      110 CL=SQRT(GAMMAL*PL/RL)
184      X=(UL-CL)*DT
185      IF(XI .GE. X) GO TO 120
      C      LEFT OF LEFT FAN
186      R=RL
187      U=UL
188      P=PL
189      GO TO 500
      C      COMPUTE CONSTANT OF ISENTROPIC LAW - A
190      120 A=PL/(RL**GAMMAL)
      C      COMPUTE DENSITY IN STATE STAR *
      C      COMPUTE SOUND SPEED IN STATE STAR *
191      RSTAR=(PSTAR/A)**(1./GAMMAL)
192      CSTAR=SQRT(GAMMAL*PSTAR/RSTAR)
193      X=(USTAR-CSTAR)*DT
194      IF(XI .GE. X) GO TO 130
      C      IN LEFT FAN
195      U=(2./(GAMMAL+1.))*(XI/DT+CL+0.5*(GAMMAL-1.)*UL)
196      RINT=CL+0.5*(GAMMAL-1.)*(UL-U)
197      R=(RINT*RINT/(A**GAMMAL))**(1./(GAMMAL-1.))
198      P=A*(R**GAMMAL)
199      GO TO 500
      C      RIGHT OF LEFT FAN
200      130 R=RSTAR
201      U=USTAR
202      P=PSTAR
203      GO TO 500
      C      RIGHT SIDE
204      200 IF(IREGR .EQ. 2) GO TO 220
      C      COMPUTE RIGHT SHOCK SPEED
205      U=UR+MR/RR
206      X=U*DT
207      IF(XI .GE. X) GO TO 210
      C      LEFT OF RIGHT SHOCK
208      R=-MR/(USTAR-U)
209      U=USTAR
210      P=PSTAR
211      GO TO 500
      C      RIGHT OF RIGHT SHOCK
212      210 R=RR
213      U=UR
214      P=PR

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215      GO TO 500
      C      COMPUTE CONSTANT OF INSENTROPIC LAW - A
216      220 A=PR/(RR**GAMMAR)
      C      COMPUTE DENSITY IN STATE STAR *
217      RSTAR=(PSTAR/A)**(1./GAMMAR)
      C      COMPUTE SOUND SPEED IN STATE STAR *
218      CSTAR=SQRT(GAMMAR*PSTAR/RSTAR)
219      X=(USTAR+CSSTAR)*DT
220      IF(XI .GE. X) GO TO 230
      C      LEFT OF RIGHT FAN
221      R=RSTAR
222      U=USTAR
223      P=PSTAR
224      GO TO 500
      C      COMPUTE SOUND SPEED IN RIGHT STATE
225      230 CR=SQRT(GAMMAR*PR/RR)
226      X=(UR+CR)*DT
227      IF(XI .GE. X) GO TO 240
      C      IN RIGHT FAN
228      U=(2./((GAMMAR+1.))*(XI/DT-CR+0.5*(GAMMAR-1.)*UR)
229      RINT=CR+0.5*(GAMMAR-1.)*(U-UR)
230      R=(RINT*RINT/(A*GAMMAR))**(1./((GAMMAR-1.))
231      P=A*(R**GAMMAR)
232      GO TO 500
      C      RIGHT OF RIGHT FAN
233      240 R=RR
234      U=UR
235      P=PR
236      500 CONTINUE
237      RETURN
238      END

```

```

239      SUBROUTINE RANDU(IX,IY,YFL)
240      IY=IX*65539
241      IF(IY)5,6,6
242      5 IY=IY+2147483647+1
243      6 YFL=IY
244      YFL=YFL*.4656613E-9
245      IX=IY
246      RETURN
247      END

248      SUBROUTINE STTOUT
249      COMMON//DT,RL,UL,PL,R,U,P,E,RR,UR,PR,XI,Y,GAMMAL,GAMMAR
250      COMMON/OUT/TIME,N,DX,RHO(301),PRE(301),UX(301),ENG(301),GAMMA(301)
251      WRITE(6,10000) TIME
252      10000 FORMAT(1H1,7H TIME = ,F11.7)
253      WRITE(6,10001)
254      10001 FORMAT(1H0,3H X,4X,5HDENSE,4X,3HVEL,5X,4HPRES,3X,3HGAM/)
255      DO 20 I=2,61
256      KT1=I-1
257      RT1=RHO(I)
258      UT1=UX(I)
259      PT1=PRE(I)
260      G1=GAMMA(I)
261      KT2=I+59
262      RT2=RHO(I+60)
263      UT2=UX(I+60)
264      PT2=PRE(I+60)
265      G2=GAMMA(I+60)
266      KT3=I+119
267      RT3=RHO(I+120)
268      UT3=UX(I+120)
269      PT3=PRE(I+120)
270      G3=GAMMA(I+120)
271      PRINT5,KT1,RT1,UT1,PT1, G1,KT2,RT2,UT2,PT2, G2,KT3,RT3,UT3,PT3, G3
272      5 FORMAT(1H ,3(I4,4F8.3,4X))
273      20 CONTINUE
274      RETURN
275      END

```



```

276      FUNCTION PHI(X,GAMMA)
277      EPS=1.0E-6
278      IF (ABS(1.-X) .GT. EPS) GO TO 100
279      PHI=SQRT(GAMMA)
280      RETURN
281 100    COEF1=0.5*(GAMMA+1.)
282      COEF2=0.5*(GAMMA-1.)
283      COEF3=COEF2/GAMMA
284      IF (X .GE. 1.) GO TO 200
285      PHI=COEF2*(1.-X)/(SQRT(GAMMA)*(1.-(X**COEF3)))
286      RETURN
287 200    PHI=SQRT(COEF1*X+COEF2)
288      RETURN
289      END

290      SUBROUTINE INHOM
291      COMMON/DT,RL,UL,PL,R,U,P,E,RR,UR,PR,XI,Y,GAMMAL,GAMMAR
292      COMMON/OUT/TIME,N,DX,RHO(301),PRE(301),UX(301),ENG(301),GAMMA(301)
293      COMMON/RAD/ETA
294      REAL MOM
295      NP1=N+1
296      DO 100 I=2,NP1
297      G=GAMMA(I)
298      X=FLOAT(I-1)*DX
299      R=RHO(I)
300      P=PRE(I)
301      U=UX(I)
302      E=P/(G-1.)+0.5*R*U*U
303      DEN=R-DT*(ETA-1.)*R*U/X
304      MOM=R*U*(1.-DT*(ETA-1.)*U/X)
305      E=E-DT*(ETA-1.)*U*(E+P)/X
306      RHO(I)=DEN
307      UX(I)=MOM/DEN
308      PRE(I)=(G-1.)*(E-0.5*MOM*MOM/DEN)
309 100    CONTINUE
310      RETURN
311      END

```

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TABLE 1. COMPARISON OF PRESENT CALCULATION WITH REF. 11

| Region | REF. 11 |        |       | PRESENT RESULTS |        |       |
|--------|---------|--------|-------|-----------------|--------|-------|
|        | $\rho$  | $p$    | $u$   | $\rho$          | $p$    | $u$   |
| 1      | 1.000   | 1.000  | 0.000 | 1.000           | 1.000  | 0.000 |
| 2      | 2.555   | 4.161  | 1.172 | 2.555           | 4.160  | 1.172 |
| 3      | 7.100   | 4.161  | 1.172 | 7.098           | 4.160  | 1.172 |
| 4      | 27.000  | 27.000 | 0.000 | 27.000          | 27.000 | 0.000 |
| 5      | 5.587   | 13.221 | 0.000 | 5.586           | 13.217 | 0.000 |
| 6      | 6.701   | 17.063 | 0.286 | 6.698           | 17.055 | 0.286 |
| 7      | 17.997  | 17.063 | 0.286 | 17.987          | 17.055 | 0.286 |
| 8      | 7.985   | 21.823 | 0.000 | 7.981           | 21.812 | 0.000 |
| 9      | 8.324   | 23.133 | 0.069 | 8.320           | 23.120 | 0.069 |
| 10     | 22.349  | 23.133 | 0.069 | 22.335          | 23.120 | 0.069 |
| 11     | 8.675   | 24.509 | 0.000 | 8.670           | 24.494 | 0.000 |
| 12     | 8.761   | 24.852 | 0.017 | 8.757           | 24.837 | 0.017 |
| 13     | 23.523  | 24.852 | 0.017 | 23.507          | 24.37  | 0.017 |
| 14     | 8.849   | 25.200 | 0.000 | 8.844           | 25.184 | 0.000 |

TABLE 2. VALUES OF  $\rho$ ,  $p$  AND  $u$  FOR REGIONS IN FIG. 5

| Region | $\rho$ | $p$    | $u$     | Region | $\rho$ | $p$    | $u$     |
|--------|--------|--------|---------|--------|--------|--------|---------|
| 2      | 2.555  | 4.160  | - 1.172 | 36     | 8.886  | 25.353 | 0.000   |
| 3      | 7.098  | 4.160  | - 1.172 | 37     | 8.818  | 25.083 | + 0.013 |
| 5      | 5.586  | 13.217 | 0.000   | 38     | 8.824  | 25.103 | + 0.012 |
| 6      | 6.698  | 17.055 | - 0.286 | 39     | 23.686 | 25.103 | + 0.012 |
| 7      | 17.987 | 17.055 | - 0.286 | 40     | 23.670 | 25.079 | + 0.013 |
| 8      | 7.981  | 21.812 | 0.000   | 41     | 23.665 | 25.073 | + 0.013 |
| 9      | 8.320  | 23.120 | - 0.069 | 42     | 23.663 | 25.072 | + 0.013 |
| 10     | 22.335 | 23.120 | - 0.069 | 43     | 23.662 | 25.071 | + 0.013 |
| 11     | 22.104 | 22.790 | - 0.058 | 44     | 22.414 | 25.071 | + 0.013 |
| 12     | 20.939 | 22.790 | - 0.058 | 45     | 22.355 | 24.979 | + 0.015 |
| 13     | 8.670  | 24.494 | 0.000   | 46     | 8.819  | 25.084 | + 0.013 |
| 14     | 8.757  | 24.837 | - 0.017 | 47     | 23.673 | 25.084 | + 0.013 |
| 15     | 23.507 | 24.837 | - 0.017 | 48     | 23.669 | 25.079 | + 0.013 |
| 16     | 23.269 | 24.487 | - 0.007 | 49     | 23.668 | 25.078 | + 0.013 |
| 17     | 23.251 | 24.463 | - 0.006 | 50     | 23.666 | 25.076 | + 0.013 |
| 18     | 22.025 | 24.463 | - 0.006 | 51     | 8.751  | 24.814 | 0.000   |
| 19     | 21.965 | 24.373 | - 0.003 | 52     | 8.756  | 24.835 | - 0.001 |
| 20     | 21.631 | 24.373 | - 0.003 | 53     | 8.752  | 24.816 | - 0.000 |
| 21     | 8.844  | 25.184 | 0.000   | 54     | 8.735  | 24.752 | + 0.003 |
| 22     | 8.865  | 25.269 | - 0.004 | 55     | 23.449 | 24.752 | + 0.003 |
| 23     | 23.798 | 25.269 | - 0.004 | 56     | 23.445 | 24.746 | + 0.003 |
| 24     | 23.558 | 24.913 | + 0.006 | 57     | 23.442 | 24.745 | + 0.003 |
| 25     | 23.541 | 24.889 | + 0.007 | 58     | 8.761  | 24.855 | 0.000   |
| 26     | 23.535 | 24.883 | + 0.007 | 59     | 8.757  | 24.837 | + 0.001 |
| 27     | 22.294 | 24.883 | + 0.007 | 60     | 8.741  | 24.772 | + 0.004 |
| 28     | 22.235 | 24.792 | + 0.010 | 61     | 8.742  | 24.777 | + 0.003 |
| 29     | 8.798  | 24.999 | + 0.008 | 62     | 23.466 | 24.777 | + 0.003 |
| 30     | 23.616 | 24.999 | + 0.008 | 63     | 23.462 | 24.771 | + 0.004 |
| 31     | 23.599 | 24.975 | + 0.009 | 64     | 8.732  | 24.818 | 0.000   |
| 32     | 23.594 | 24.969 | + 0.009 | 65     | 8.736  | 24.754 | + 0.003 |
| 33     | 23.592 | 24.968 | + 0.010 | 66     | 8.737  | 24.759 | + 0.003 |
| 34     | 22.348 | 24.968 | + 0.010 | 67     | 8.719  | 24.690 | 0.000   |
| 35     | 22.289 | 24.876 | + 0.013 | 68     | 8.721  | 24.694 | - 0.000 |

TABLE 3. COMPARISON OF PRESENT CALCULATIONS WITH REF. 12

| Region | REF. 12 |         |         | PRESENT RESULTS |         |        |
|--------|---------|---------|---------|-----------------|---------|--------|
|        | $\rho$  | $p$     | $u$     | $\rho$          | $p$     | $u$    |
| 0      | 1.00000 | 1.00000 | 0.00000 | 1.0000          | 1.0000  | 0.0000 |
| 1      | 1.60300 | 1.96000 | 0.50789 | 1.603           | 1.960   | 0.5079 |
| 2      | 0.64340 | 0.53935 | 0.42207 | 0.6435          | 0.5393  | 0.4217 |
| 3      | 1.07360 | 1.12217 | 0.93126 | 1.074           | 1.122   | 0.9314 |
| 4      | 1.07630 | 1.12217 | 0.93126 | 1.076           | 1.122   | 0.9314 |
| 5      | 2.42830 | 1.96000 | 0.50789 | 2.428           | 1.960   | 0.5079 |
| 6      | 0.45660 | 0.53935 | 0.42207 | 0.4565          | 0.5393  | 0.4217 |
| 7      | 4.41850 | 4.1485  | 0.00000 | 4.1485          | 4.1485  | 0.0000 |
| 8      | 0.30659 | 0.30659 | 0.00000 | 0.30659         | 0.30659 | 0.0000 |

TABLE 4. HEAD-ON COLLISION OF TWO RAREFACTION WAVES

| Region | METHOD OF CHARACTERISTICS |          |          | PRESENT NUMERICAL RESULTS |          |         |
|--------|---------------------------|----------|----------|---------------------------|----------|---------|
|        | $\rho$                    | $p$      | $u$      | $\rho$                    | $p$      | $u$     |
| 1      | 0.49119                   | 0.024793 | 0.0000   | 0.49119                   | 0.024793 | 0.000   |
| 2      | 1.5984                    | 0.3995   | 0.6145   | 1.598                     | 0.399    | 0.614   |
| 3      | 0.5192                    | 0.3995   | 0.6145   | 0.519                     | 0.399    | 0.614   |
| 4      | 1.0000                    | 1.0000   | 0.0000   | 1.000                     | 1.000    | 0.0     |
| 5      | 0.6901                    | 0.5950   | - 0.3576 | 0.690                     | 0.595    | - 0.358 |
| 6      | 4.5474                    | 0.5950   | - 0.3576 | 4.547                     | 0.595    | - 0.358 |
| 7      | 1.7457                    | 0.088118 | 0.0000   | 1.7457                    | 0.088118 | 0.000   |
| 8      | 0.3393                    | 0.2202   | 0.2569   | 0.339                     | 0.220    | 0.257   |

TABLE 5. CONTACT-SURFACE TAILORING

| Region | EXACT SOLUTIONS |        |       | PRESENT NUMERICAL RESULTS |        |       |
|--------|-----------------|--------|-------|---------------------------|--------|-------|
|        | $\rho$          | $p$    | $u$   | $\rho$                    | $p$    | $u$   |
| 1      | 1.000           | 1.000  | 0.000 | 1.000                     | 1.000  | 0.000 |
| 2      | 3.100           | 12.310 | 2.140 | 3.079                     | 12.310 | 2.141 |
| 3      | 3.484           | 12.310 | 2.140 | 3.484                     | 12.310 | 2.141 |
| 4      | 10.568          | 58.207 | 0.000 | 10.568                    | 58.207 | 0.000 |
| 5      | 6.907           | 54.982 | 0.000 | 6.860                     | 54.976 | 0.000 |
| 7      | 6.907           | 54.982 | 0.000 | 6.860                     | 54.976 | 0.000 |
| 8      | 9.253           | 54.982 | 0.000 | 9.251                     | 54.976 | 0.000 |

TABLE 6. SHOCK-WAVE REFRACTION AT A STATIONARY CONTACT LAYER

| Region | EXACT SOLUTIONS |        |        | PRESENT NUMERICAL RESULTS |       |       |
|--------|-----------------|--------|--------|---------------------------|-------|-------|
|        | $\rho$          | $p$    | $u$    | $\rho$                    | $p$   | $u$   |
| 1      | 0.13823         | 1.0000 | 0.0000 | 0.138                     | 1.000 | 0.0   |
| 2      | 0.2183          | 2.1965 | 1.5058 | 0.218                     | 2.196 | 1.505 |
| 3      | 1.6481          | 2.1965 | 1.5058 | 1.648                     | 2.196 | 1.505 |
| 4      | 2.3920          | 3.7000 | 1.0594 | 2.392                     | 3.700 | 1.059 |
| 5      | 1.0000          | 1.0000 | 0.0000 | 1.000                     | 1.000 | 0.0   |
| 6      | 1.0000          | 1.0000 | 0.0000 | 1.000                     | 1.000 | 0.0   |
| 7      | 2.0988          | 2.9717 | 0.8587 | 2.099                     | 2.971 | 0.859 |
| 8      | 0.2560          | 2.9717 | 0.8587 | 0.261                     | 2.971 | 0.859 |

TABLE A-1 RELATION BETWEEN SAMPLED REGION IN FIG. A-2 AND CONTACT-SURFACE  
MOVEMENT

|                  | SAMPLED REGION | MOVEMENT OF CONTACT SURFACE |
|------------------|----------------|-----------------------------|
| First-half step  | A              | + 1                         |
|                  | B              | 0                           |
| Second-half step | C              | 0                           |
|                  | D              | - 1                         |



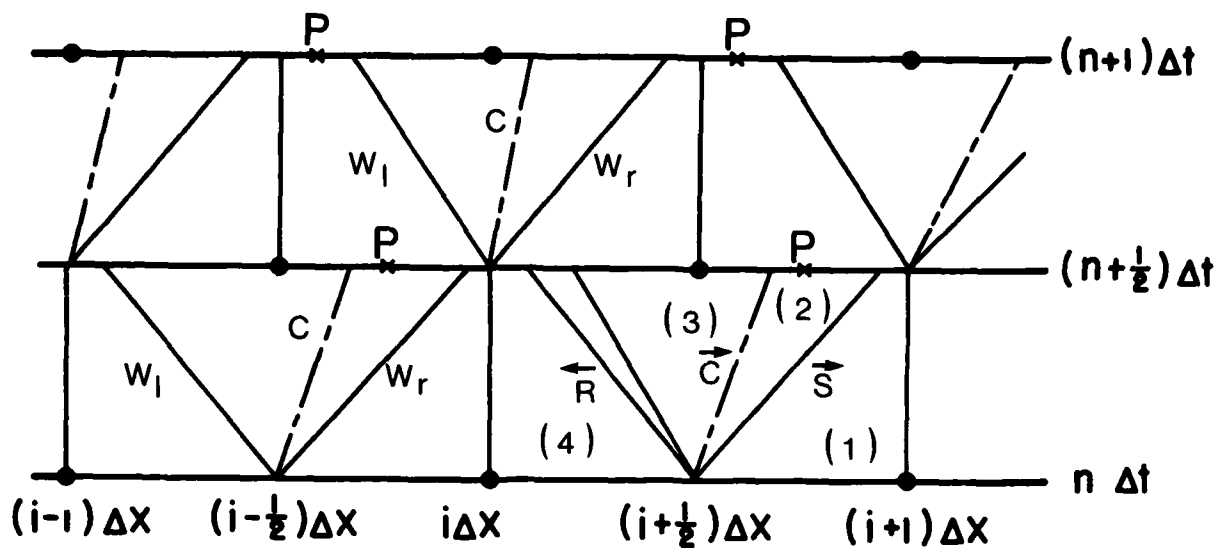


FIG. 1 GRID CONSTRUCTION FOR RANDOM-CHOICE METHOD AND SEQUENCE OF SAMPLING PROCEDURE.

● - GRID POINTS WHERE SOLUTIONS ARE SOUGHT;  $w_l$ ,  $w_r$  - LEFT OR RIGHT RUNNING WAVES;  $c$  - CONTACT SURFACE;  $P$  - SAMPLING POINT.

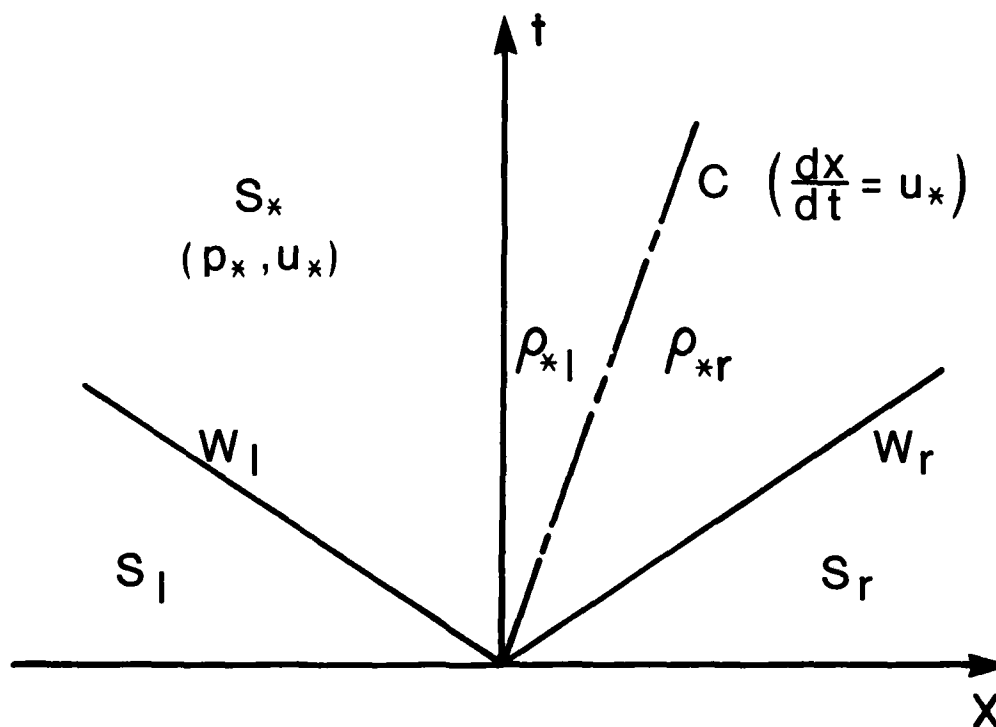


FIG. 2 SOLUTION OF A RIEMANN PROBLEM IN  $(x-t)$ -PLANE.

# Regions

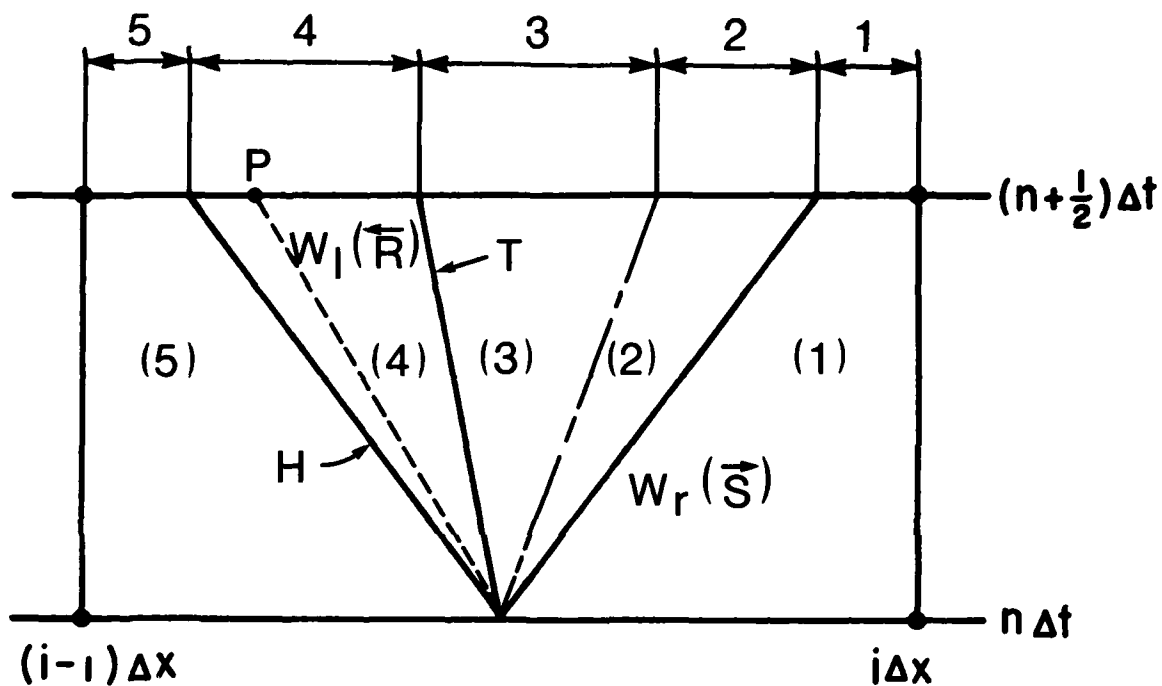


FIG. 3 FIVE DIFFERENT SOLUTIONS OF A RIEMANN PROBLEM CORRESPONDING TO THE SAMPLED REGION OR STATE.

$W_l = R$  - RAREFACTION WAVE;  $H$  - HEAD,  $T$  - TAIL;  $C$  - CONTACT SURFACE;  $W_r = S$  - SHOCK WAVE.

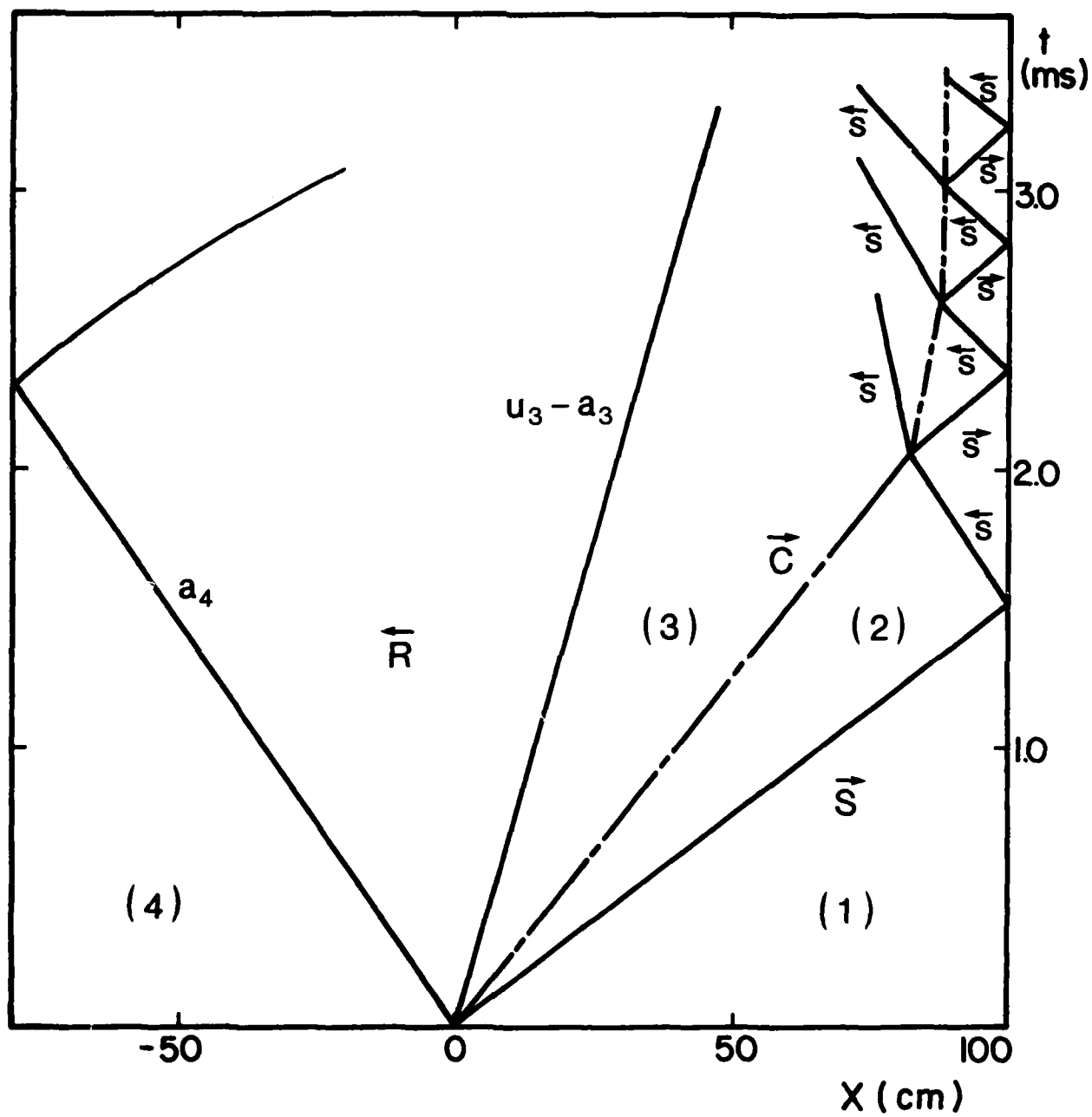


FIG. 4 WAVE DIAGRAM IN  $(x, t)$ -PLANE (REF. 11).

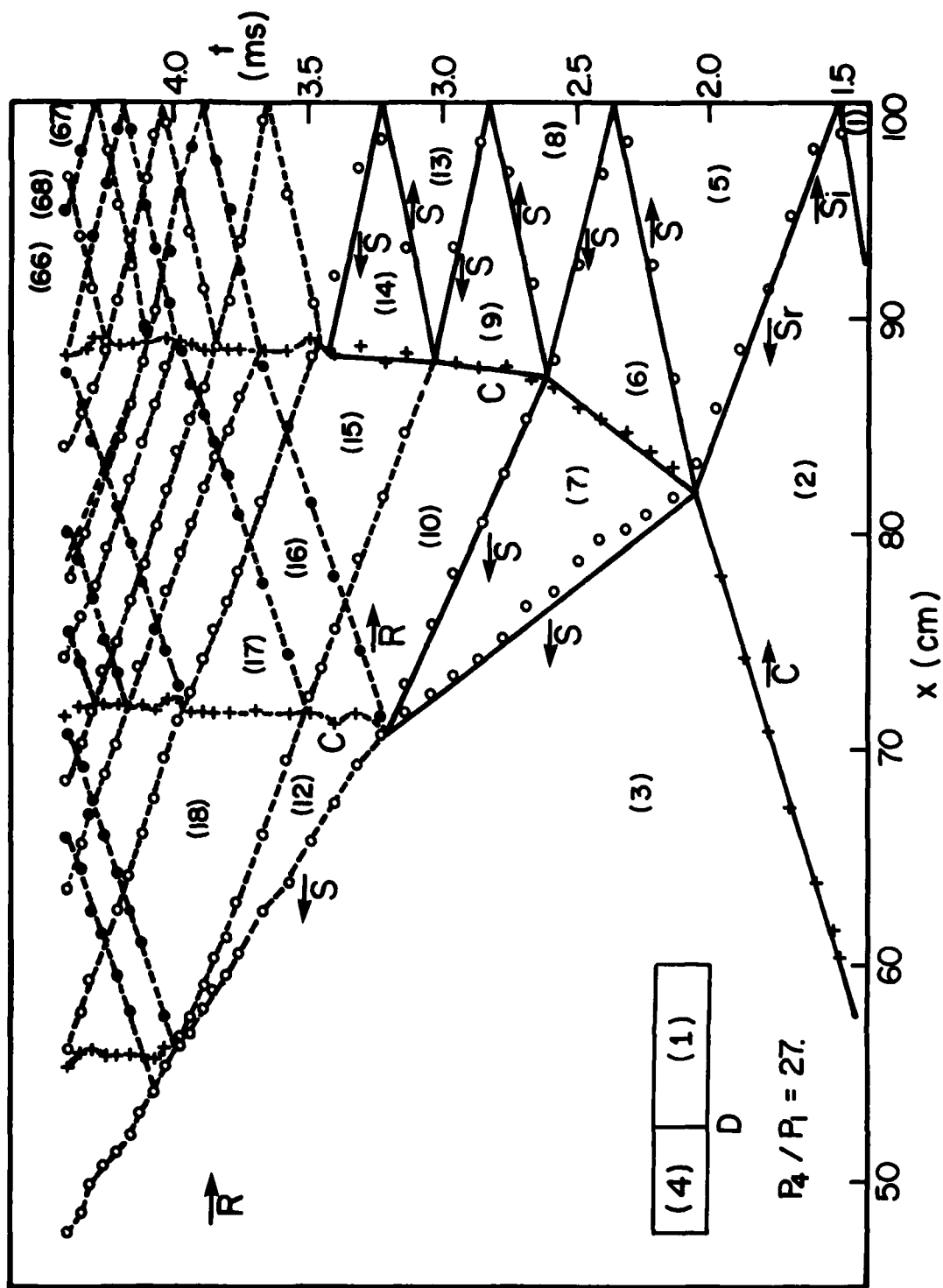


FIG. 5 DIAGRAM OF (x, t)-PLANE SHOWING A PLANE-SHOCK-WAVE REFLECTION FROM THE END WALL OF A SHOCK TUBE AND ITS SUBSEQUENT INTERACTIONS.  $p_4, p_1$  - INITIAL PRESSURES; D - DIAPHRAGM, — FROM REF. 11.

PRESENT NUMERICAL VALUES: ○ ○ ○ SHOCK WAVES; ● ● ● RAREFACTION WAVES; + + + CONTACT SURFACES.

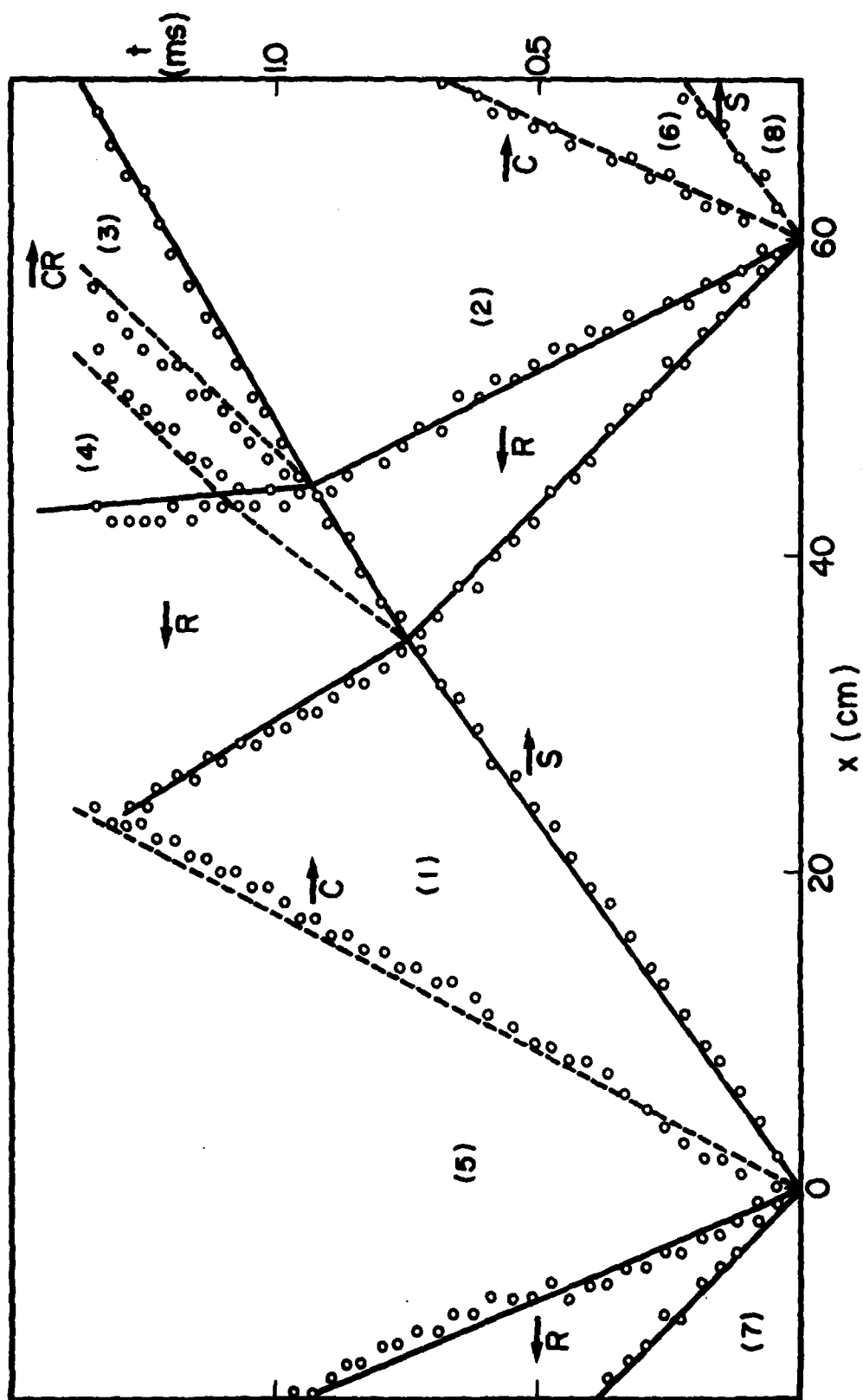


FIG. 6 HEAD-ON COLLISION OF A SHOCK WAVE WITH A RAREFACTION WAVE. O O PRESENT NUMERICAL VALUES. FROM REF. 12: — SHOCK WAVES; --- RAREFACTION WAVES; --- CONTACT SURFACES.

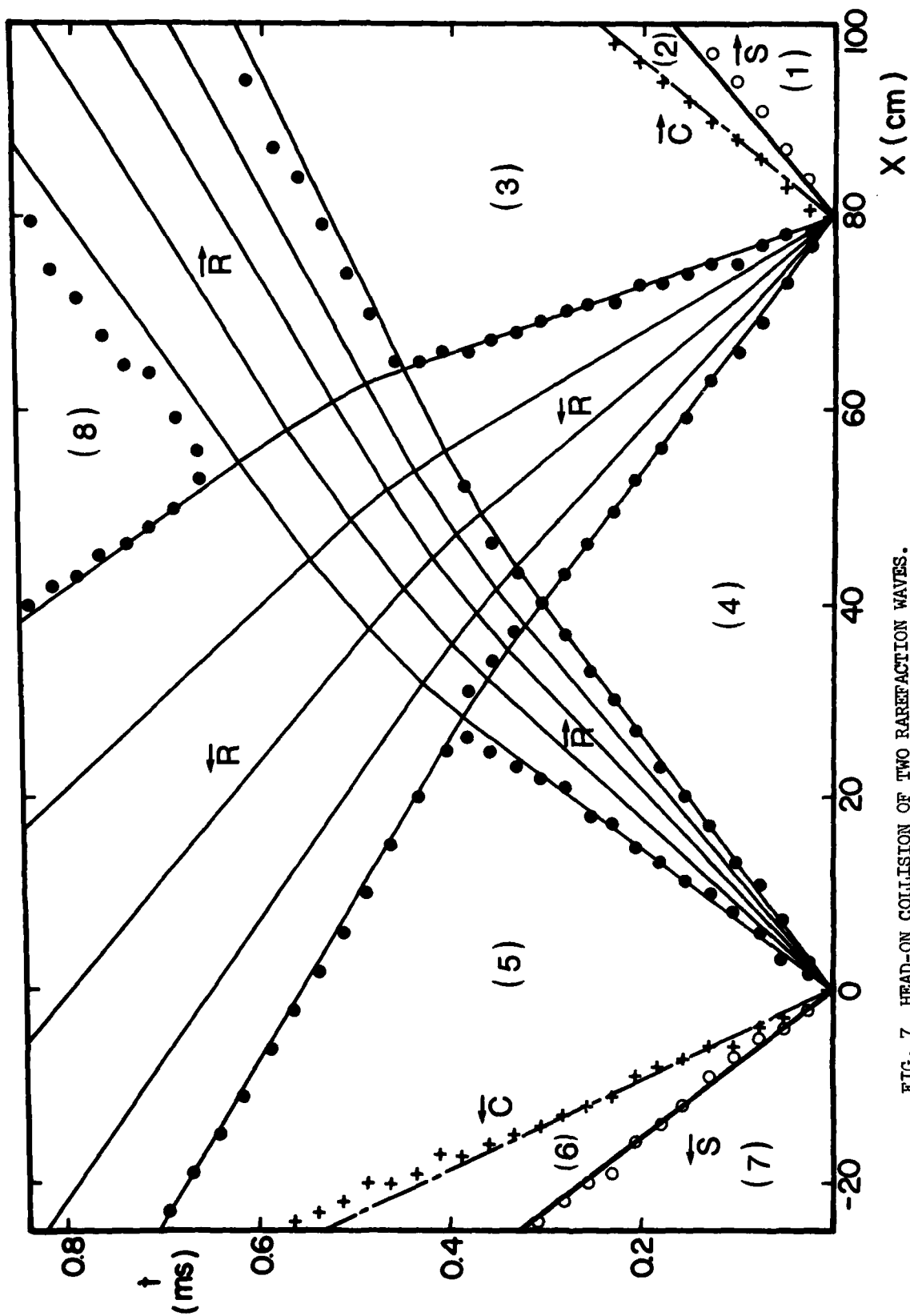


FIG. 7 HEAD-ON COLLISION OF TWO RAREFACTION WAVES.  
 INITIAL DIAPHRAGM PRESSURE RATIOS:  $p_{u1}/p_1 = 40.33$ ,  $p_{u7}/p_7 = 11.35$ .  
 — FROM REF. 13.  
 PRESENT NUMERICAL VALUES: O O SHOCK WAVES; ● ● RAREFACTION WAVES; + + + CONTACT SURFACES.

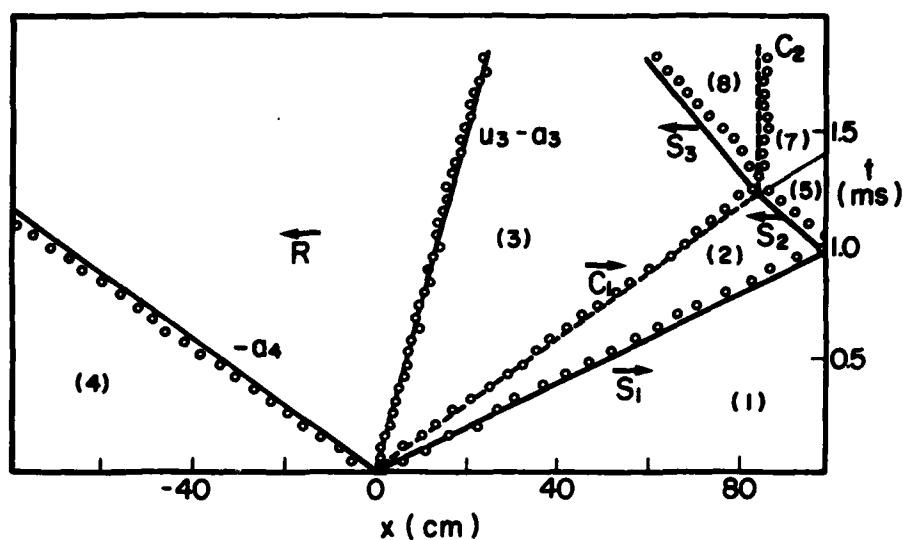


FIG. 8 NUMERICAL CONTACT-SURFACE TAILORING.

INITIAL CONDITIONS:  $p_4/p_1 = 58.207$

$\gamma_1 = 1.400$ ,  $a_1 = 322.000$  m/s

$\gamma_4 = 1.667$ ,  $a_4 = 692.548$  m/s

WAVE SPEEDS:

$M_s = S_1/a_1 = 3.1698$ ,  $M_c = C_1/a_1 = 2.1404$

$M_3 = (u_3 - a_3)/a_1 = 0.41775$ ,  $M_4 = S_2/a_1 = -1.74315$

$M_{ts} = S_2/a_1 = -1.74315$ ,  $M_{ts} = S_3/a_1 = -1.26913$

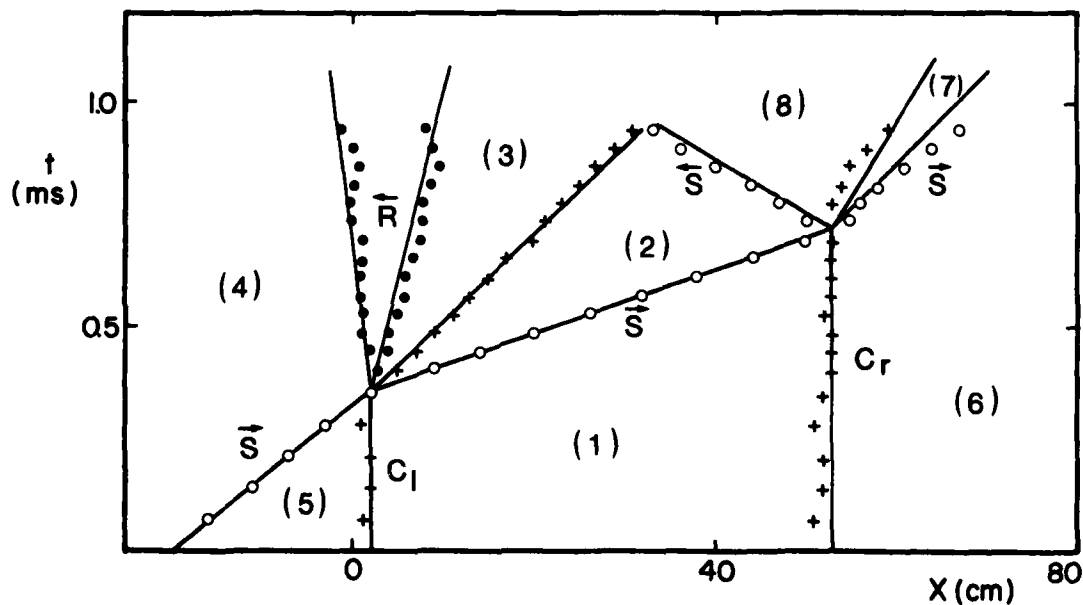


FIG. 9 SHOCK-WAVE REFRACTION AT A STATIONARY CONTACT LAYER.

INCIDENT SHOCK STRENGTH  $p_2/p_1 = 3.70$ . — FROM REF. 15.

PRESENT NUMERICAL VALUES: ○ ○ ○ SHOCK WAVES; ● ● ● RAREFACTION WAVES; + + + CONTACT SURFACES.

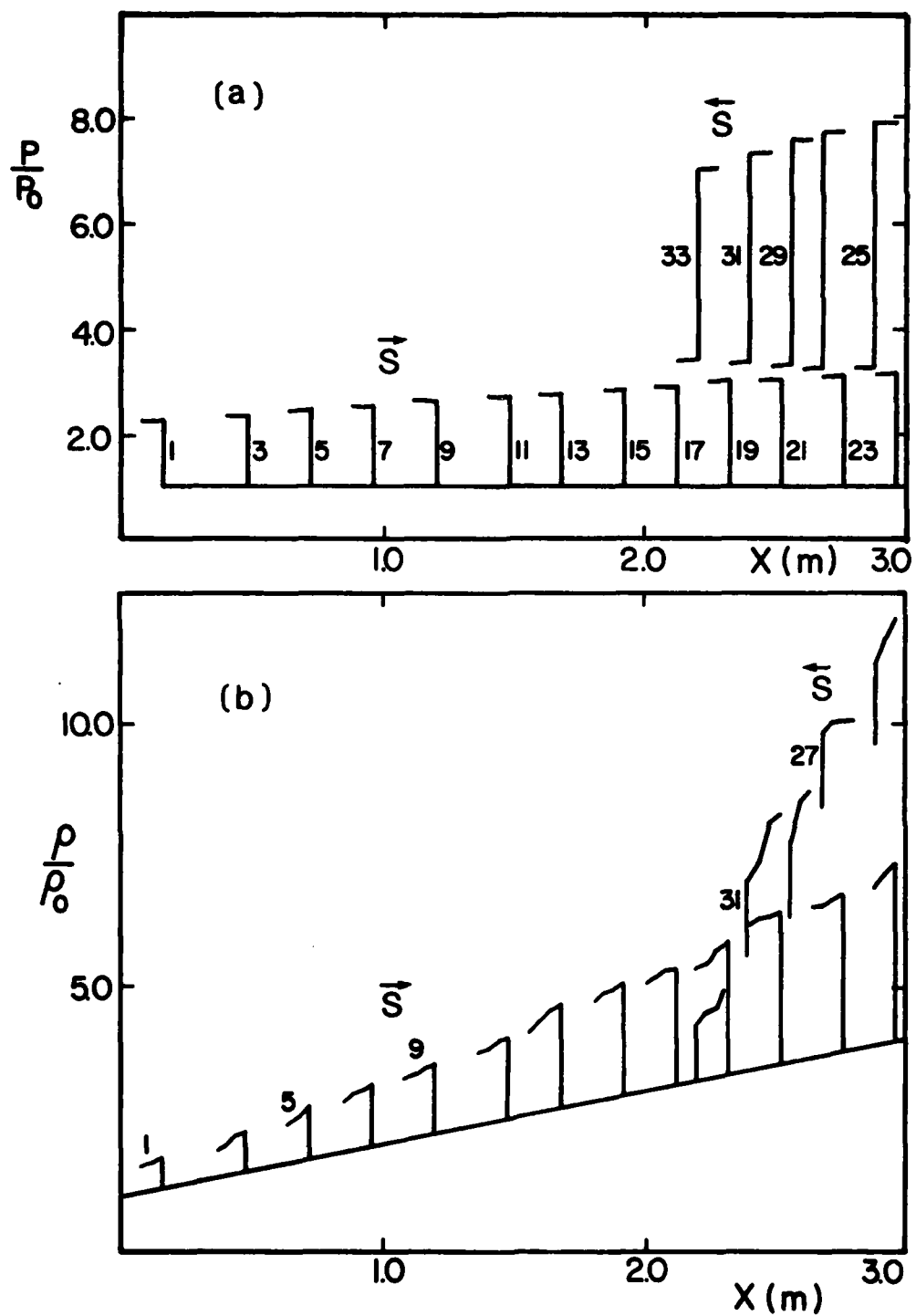


FIG. 10. PROFILES AT FIXED TIMES FOR A SHOCK WAVE MOVING IN A VARIABLE DENSITY STATE (a) PRESSURE, (b) DENSITY.

TIME NUMBERS: 1 - 0.132 ms, 3 - 0.362 ms, 5 - 0.591 ms, 7 - 0.820 ms, 9 - 1.05 ms, 11 - 1.28 ms, 13 - 1.51 ms, 15 - 1.74 ms, 17 - 1.96 ms, 19 - 2.19 ms, 21 - 2.42 ms, 23 - 2.65 ms, 25 - 2.87 ms, 27 - 3.10 ms, 29 - 3.33 ms, 31 - 3.55 ms, 33 - 3.78 ms.



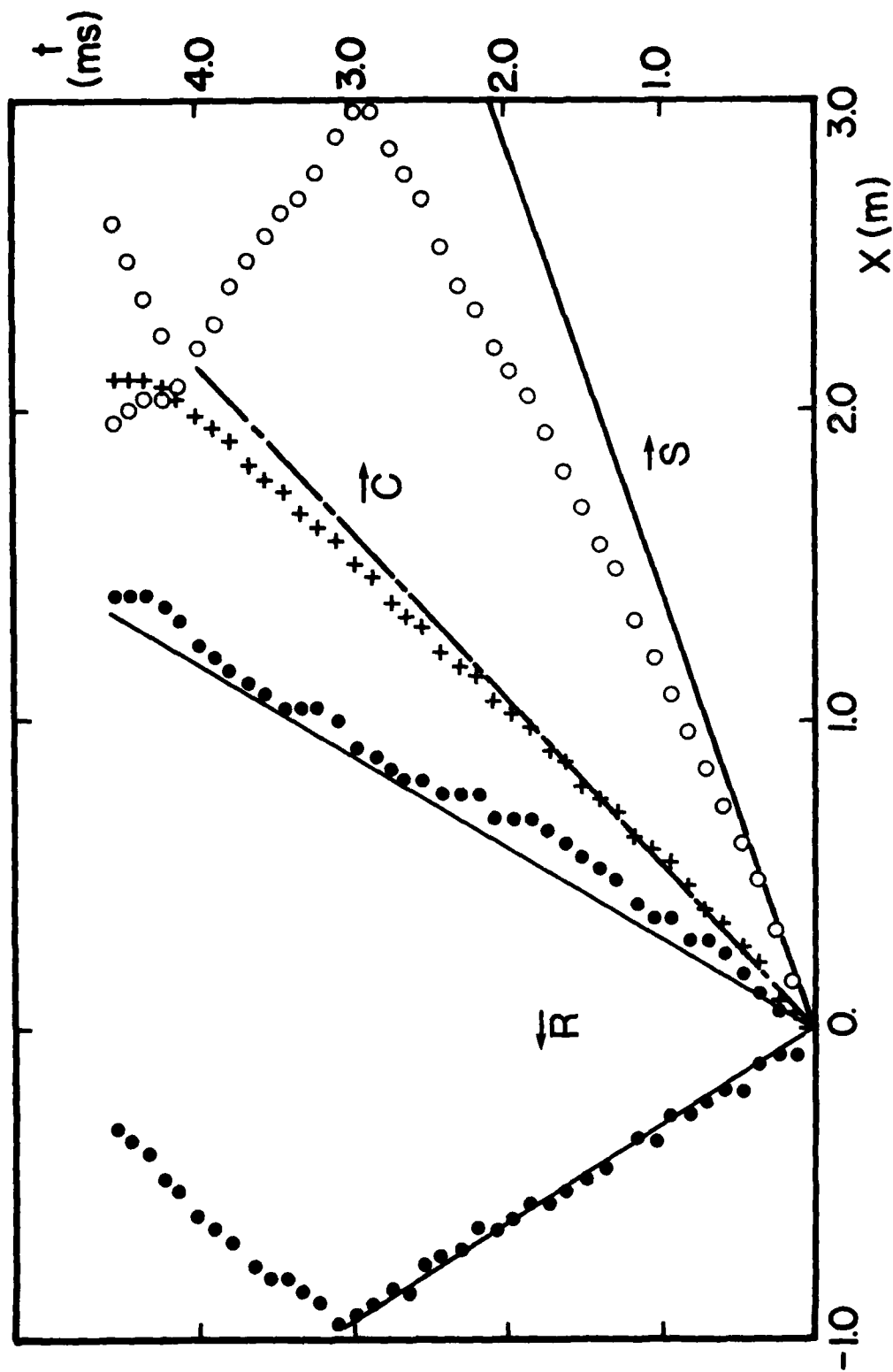


FIG. 11 WAVE DIAGRAM IN  $(x, t)$ -PLANE FOR NONUNIFORM DENSITY CHANNEL STATE IN A SHOCK TUBE.

— WAVE DIAGRAM FOR UNIFORM DENSITY FIELD.

PRESENT NUMERICAL RESULTS:  $\circ$   $\circ$  SHOCK WAVES;  $\bullet$   $\bullet$  RAREFACTION WAVES;  $+$   $+$   $+$  CONTACT SURFACES.

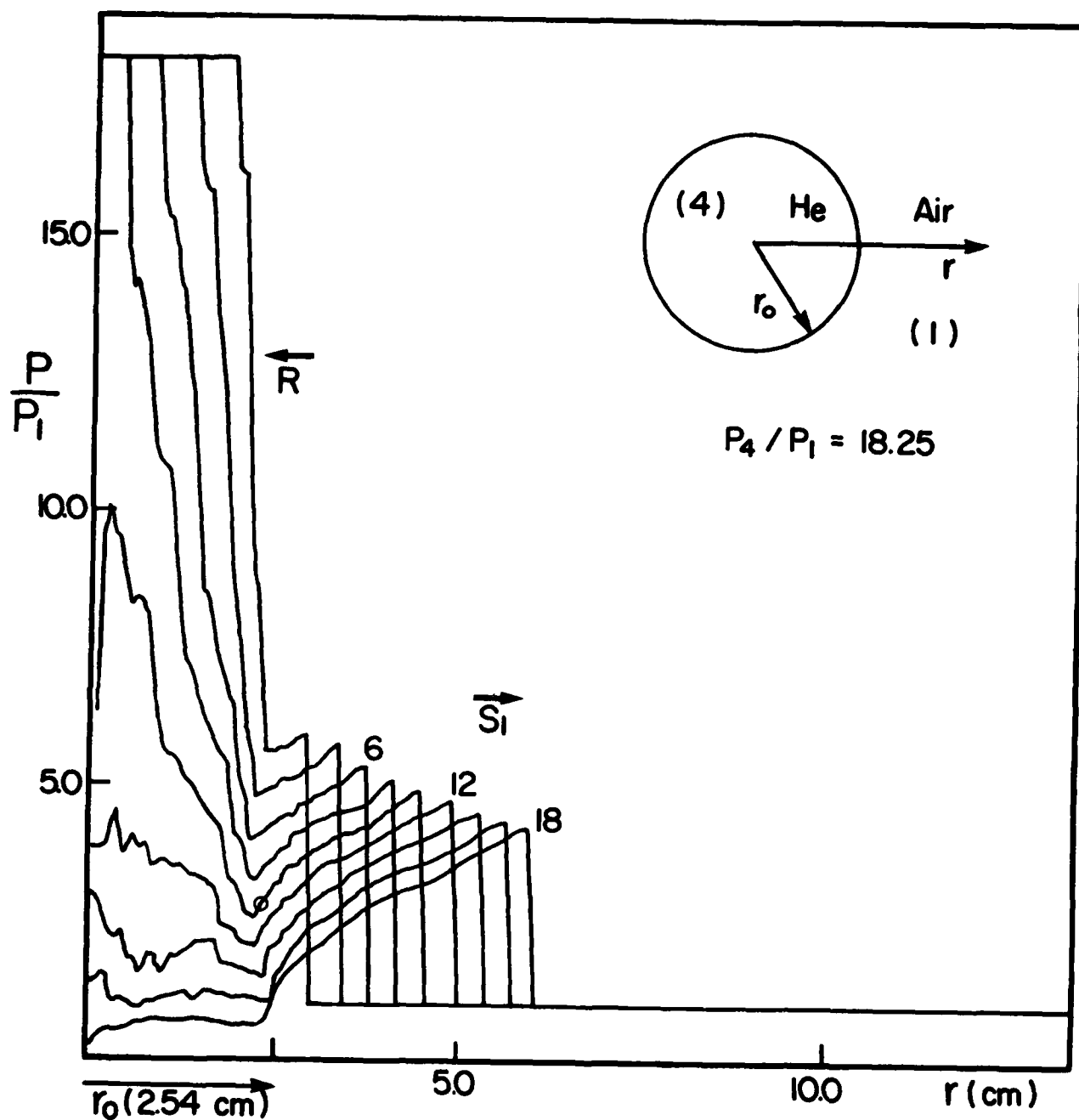


FIG. 12-a EXPLOSION OF A HELIUM SPHERE. PRESSURE PROFILES vs RADIUS FOR FIXED TIMES.  $\gamma_1 = 1.400$ ,  $\gamma_4 = 1.667$ , DIAPHRAGM PRESSURE RATIO 18.25; SHOCK MACH NUMBER  $M_s = 2.39$ , PRESSURE RATIO  $P_{21} = 6.50$ , DENSITY RATIO  $\rho_{21} = 3.20$ , PARTICLE VELOCITY  $U_{21} = 1.64$ ; THE FOREGOING ARE THE INITIAL CONDITIONS FOR THE PLANAR (SHOCK TUBE) CASE. o BIRTH POINT OF SECOND SHOCK. TIME NUMBERS: 6 - 16  $\mu s$ , 12 - 31.7  $\mu s$ , 18 - 47.2  $\mu s$ .

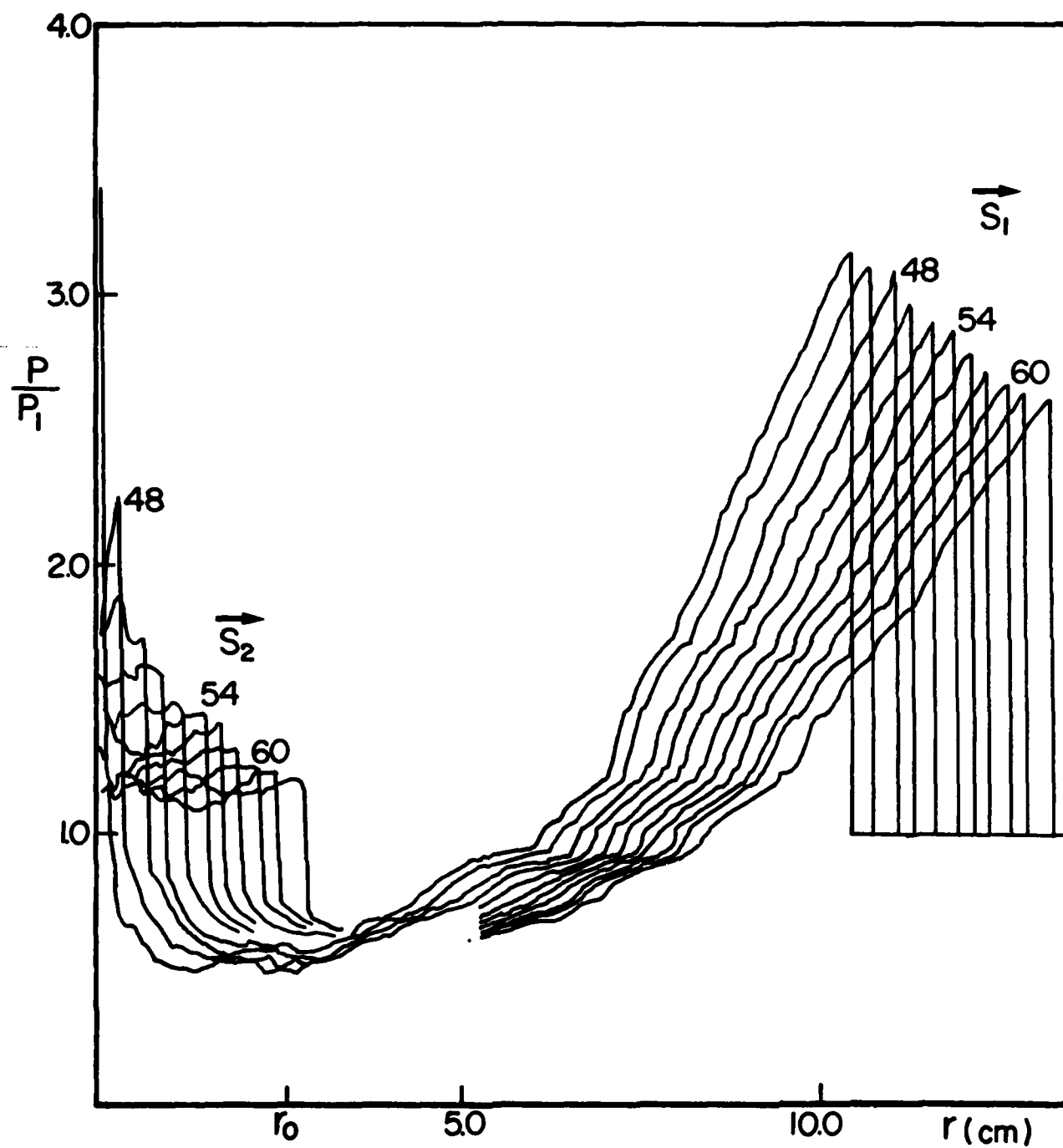


FIG. 12-b EXPLOSION OF A HELIUM SPHERE. PRESSURE PROFILES vs RADIUS FOR FIXED TIMES AFTER SECOND SHOCK WAVE IS REFLECTED. TIME NUMBERS: 48 - 125.  $\mu$ s, 54 - 140.  $\mu$ s, 60 - 156.  $\mu$ s.

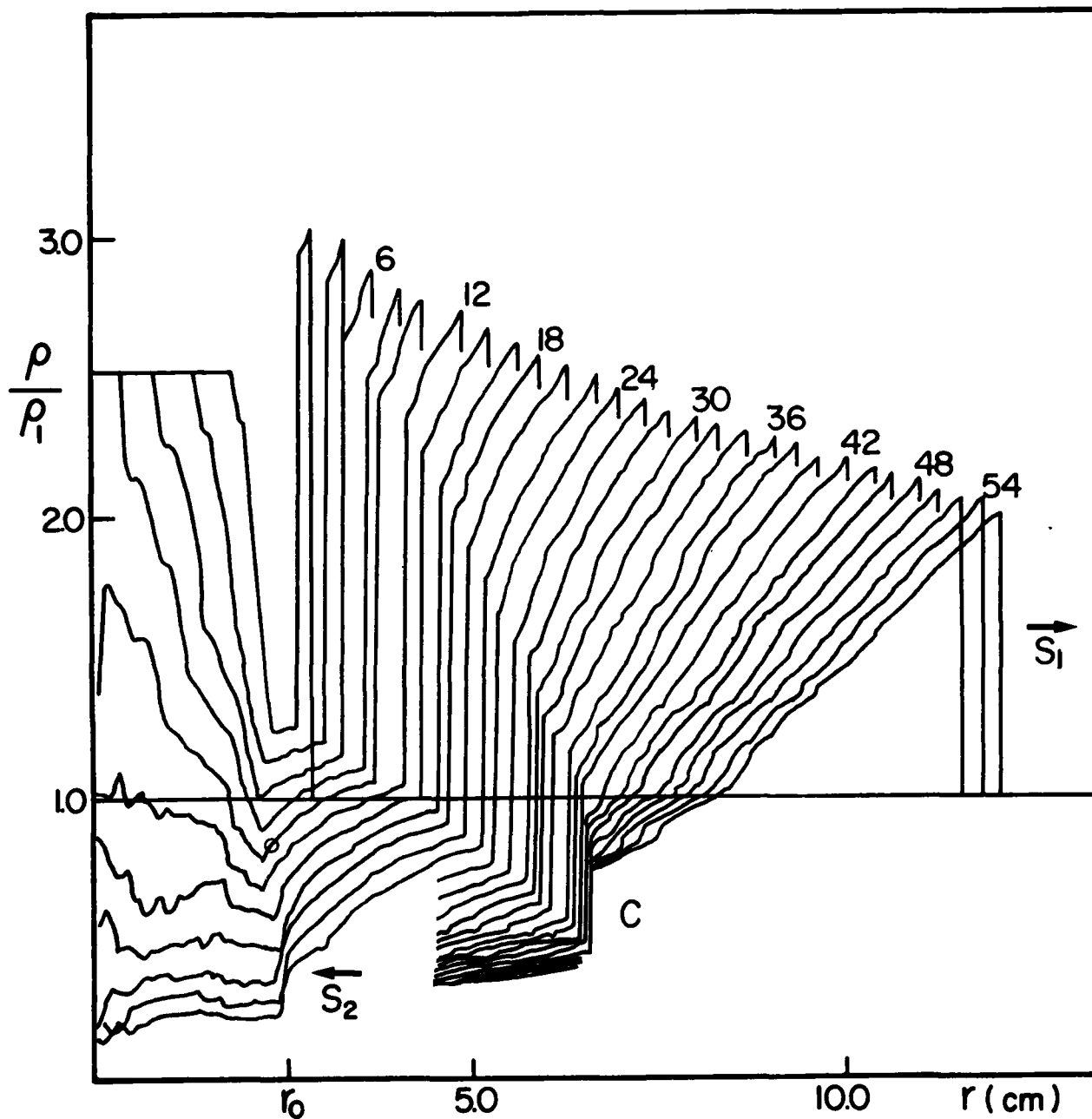


FIG. 13 EXPLOSION OF A HELIUM SPHERE. DENSITY PROFILES vs RADIUS FOR FIXED TIMES.  $\circ$  BIRTH POINT OF SECOND SHOCK. TIME NUMBERS: 6 - 16.1  $\mu$ s, 12 - 31.7  $\mu$ s, 18 - 47.2  $\mu$ s, 24 - 62.8  $\mu$ s, 30 - 78.3  $\mu$ s, 36 - 93.9  $\mu$ s, 42 - 109.  $\mu$ s, 48 - 125.  $\mu$ s, 54 - 140.  $\mu$ s.

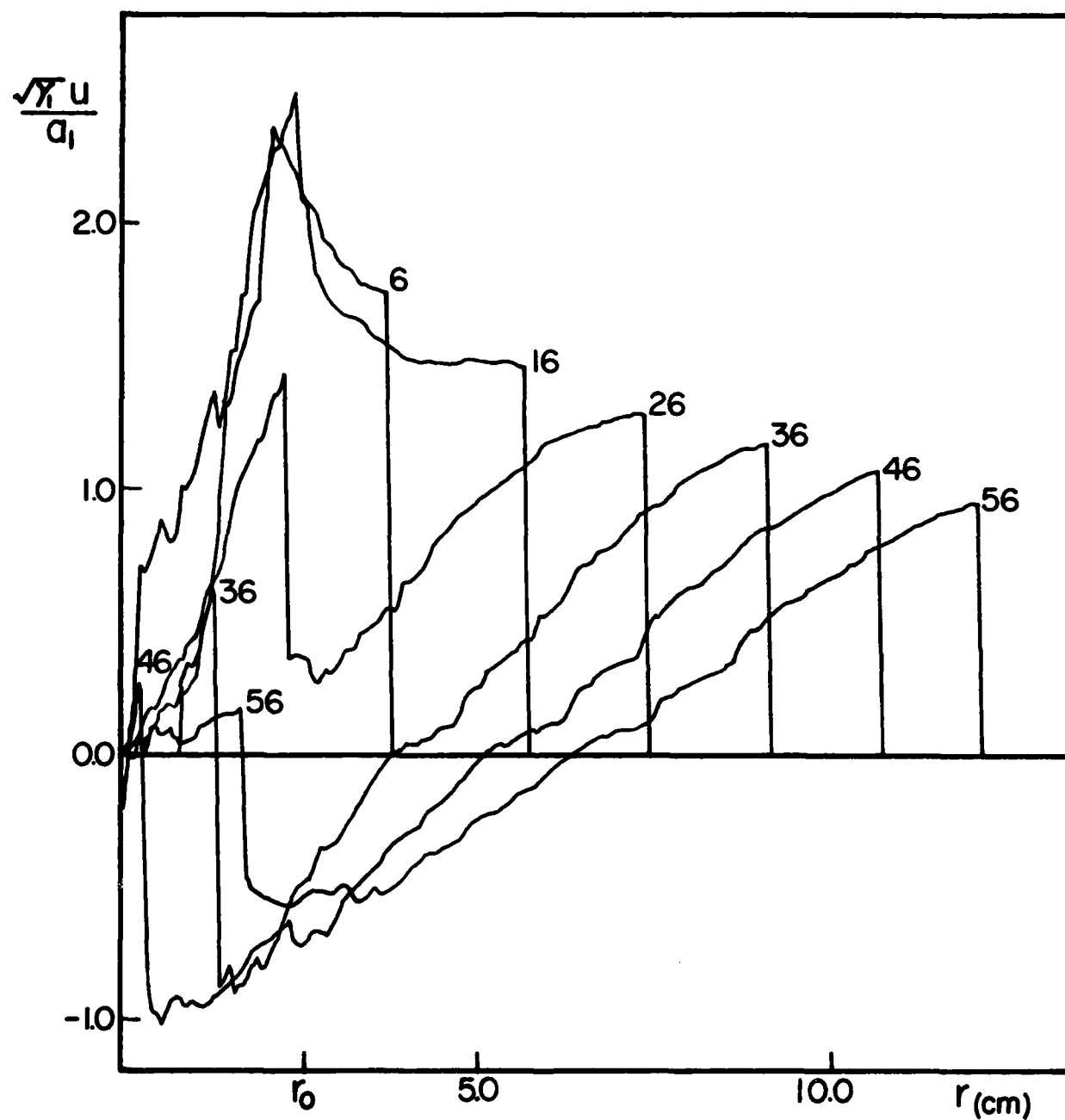


FIG. 14 EXPLOSION OF A HELIUM SPHERE. PARTICLE VELOCITY PROFILES vs RADIUS FOR FIXED TIMES. TIME NUMBERS: 6 - 16.1  $\mu$ s, 16 - 42.0  $\mu$ s, 26 - 68.0  $\mu$ s, 36 - 93.6  $\mu$ s, 46 - 120.  $\mu$ s, 56 - 146.  $\mu$ s.

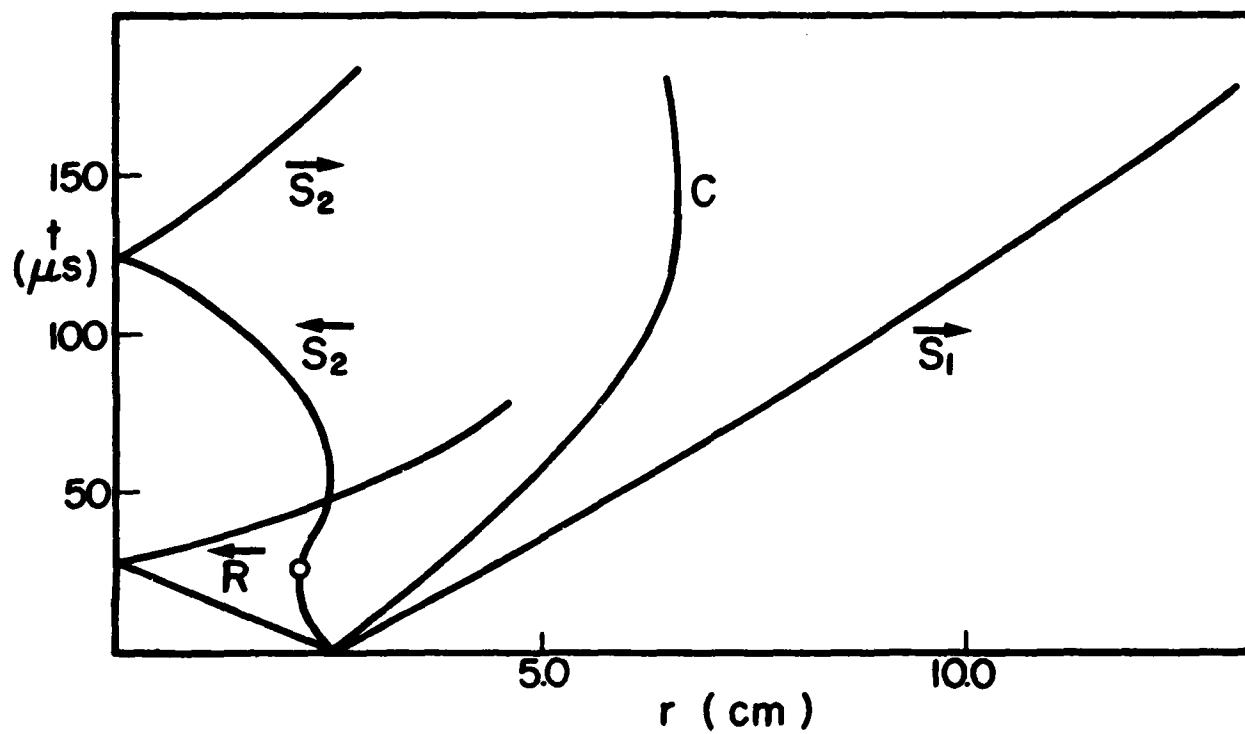


FIG. 15 EXPLOSION WAVE DIAGRAM IN THE  $(r, t)$ -PLANE.  $\circ$  BIRTH POINT OF SECOND SHOCK.

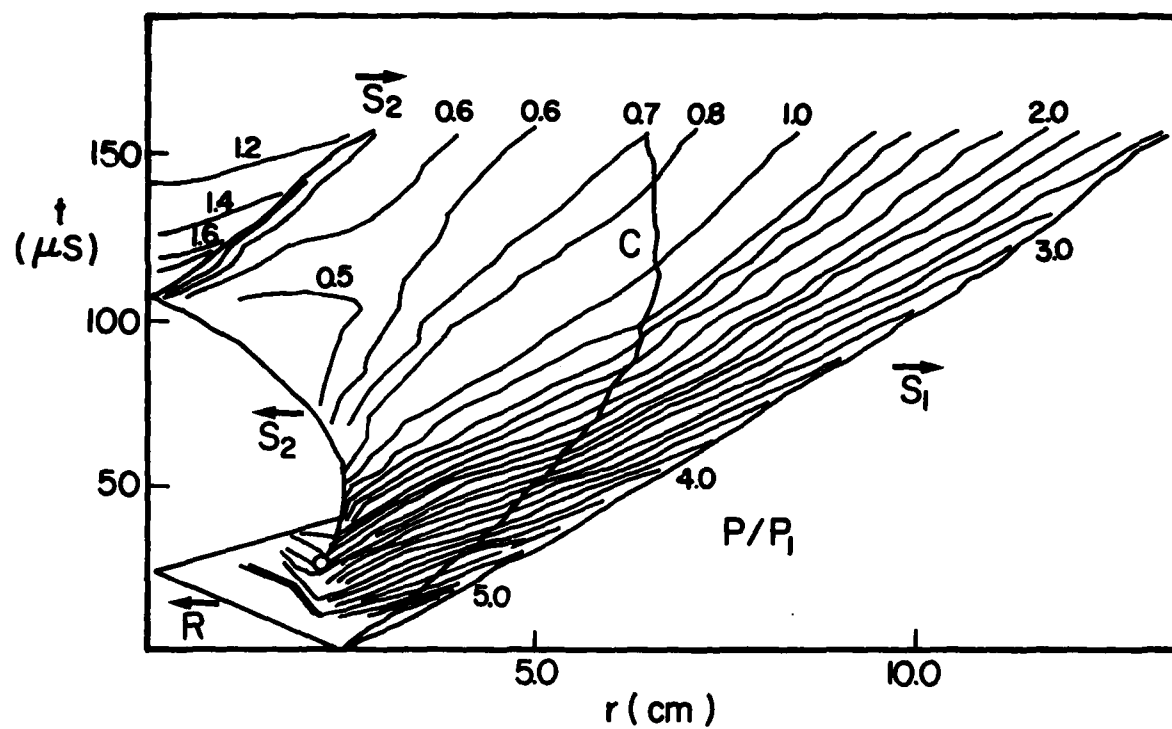


FIG. 16-a ISOBARS IN THE  $(r, t)$ -PLANE.  $\circ$  BIRTH POINT OF SECOND SHOCK.

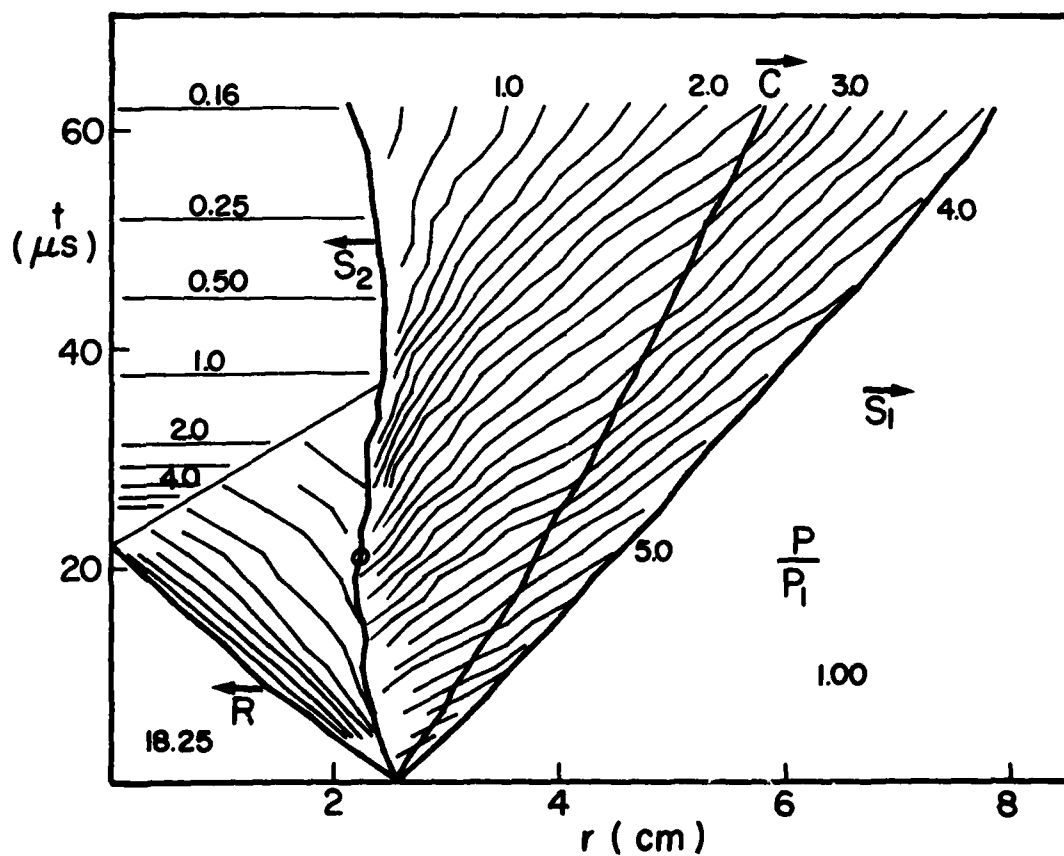


FIG. 16-b DETAILED AREA OF ISOBARS NEAR THE ORIGIN.  $\circ$  BIRTH POINT OF SECOND SHOCK.

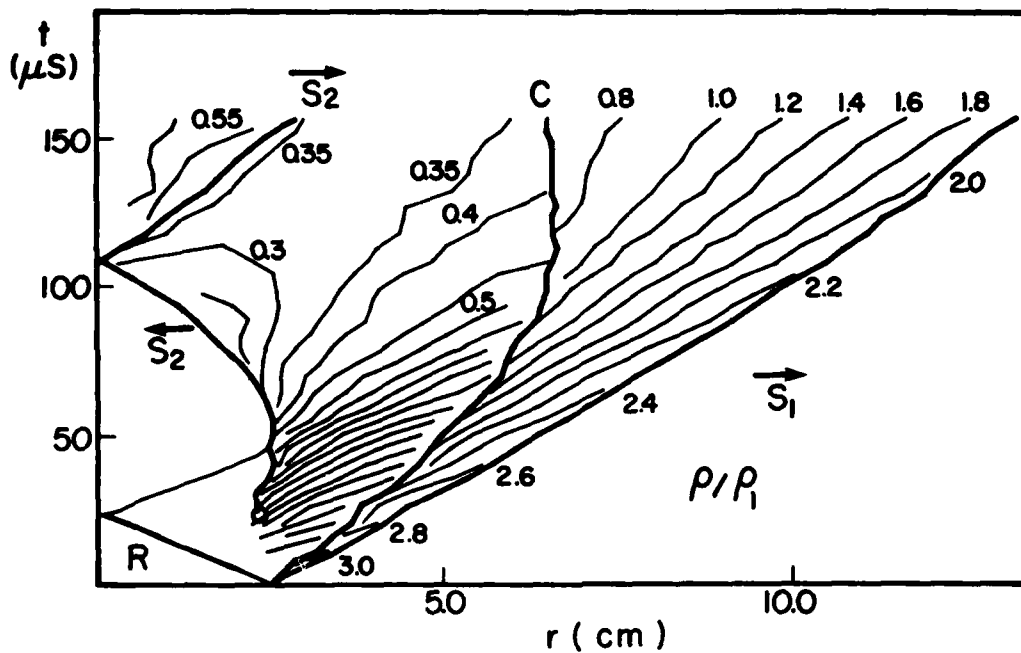


FIG. 17-a ISOPYCNICS IN THE  $(r, t)$ -PLANE.  $\circ$  BIRTH POINT OF SECOND SHOCK.

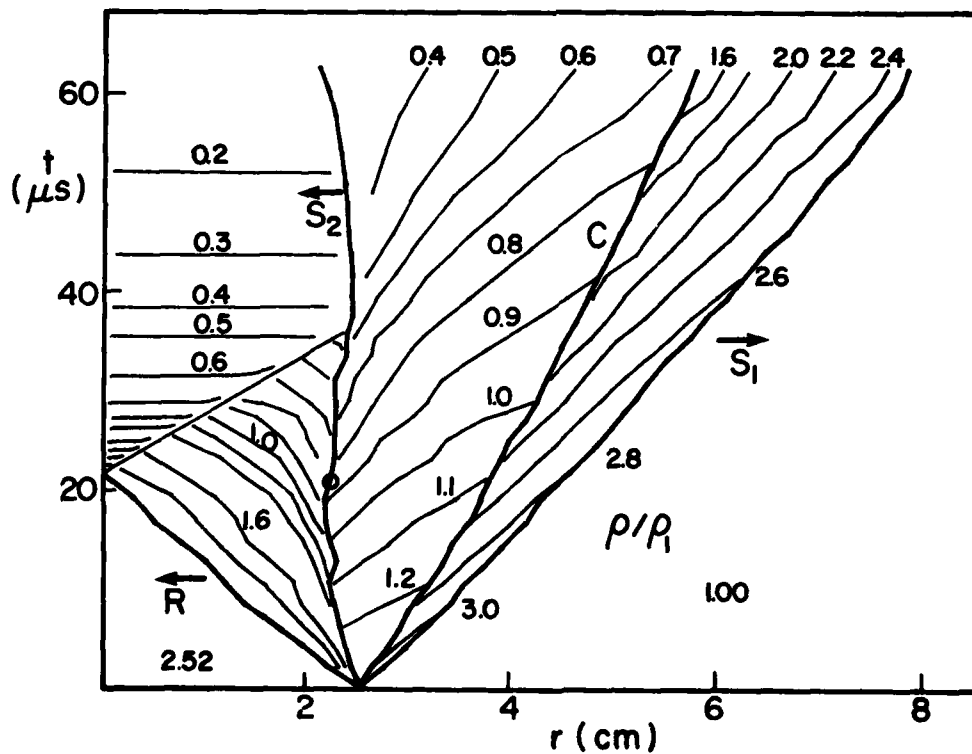


FIG. 17-b DETAILED AREA OF ISOPYCNICS NEAR THE ORIGIN.  $\circ$  BIRTH POINT OF SECOND SHOCK.



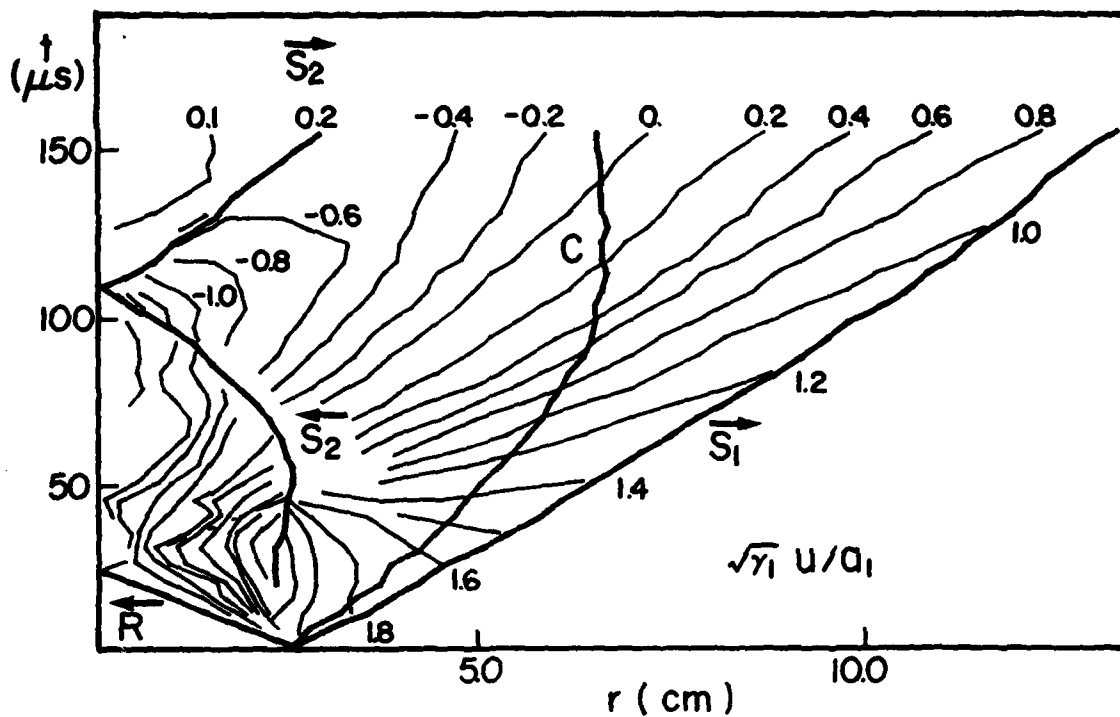


FIG. 18 ISOTACHS IN THE  $(r, t)$ -PLANE.  $\circ$  BIRTH POINT OF SECOND SHOCK.

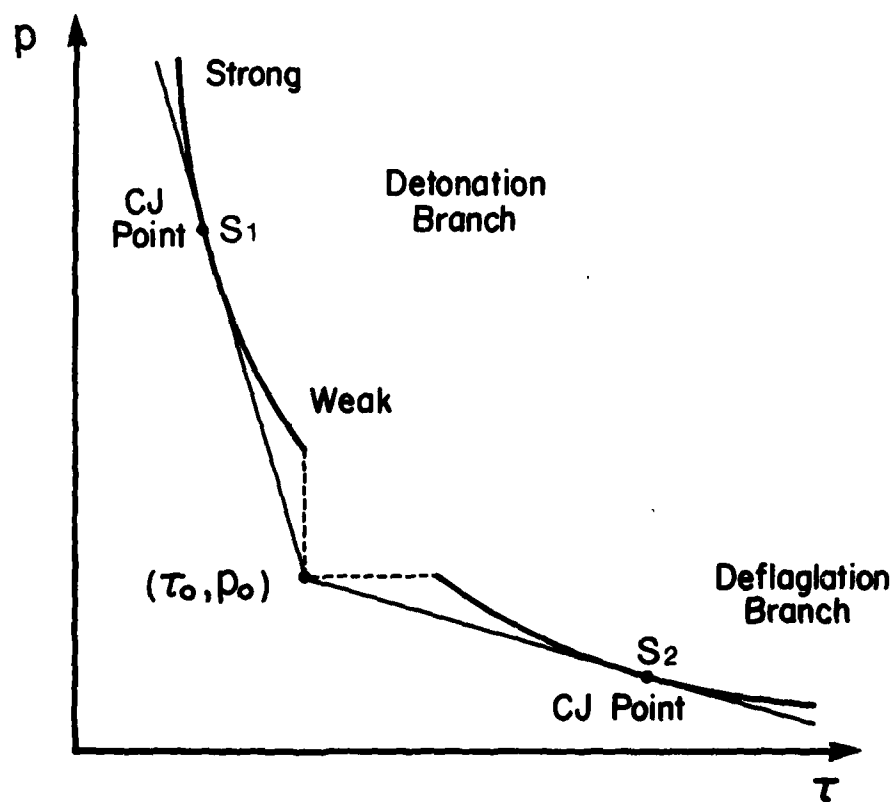


FIG. 19 THE HUGONIOT CURVE FOR EXOTHERMIC GAS FLOW (REF. 7).

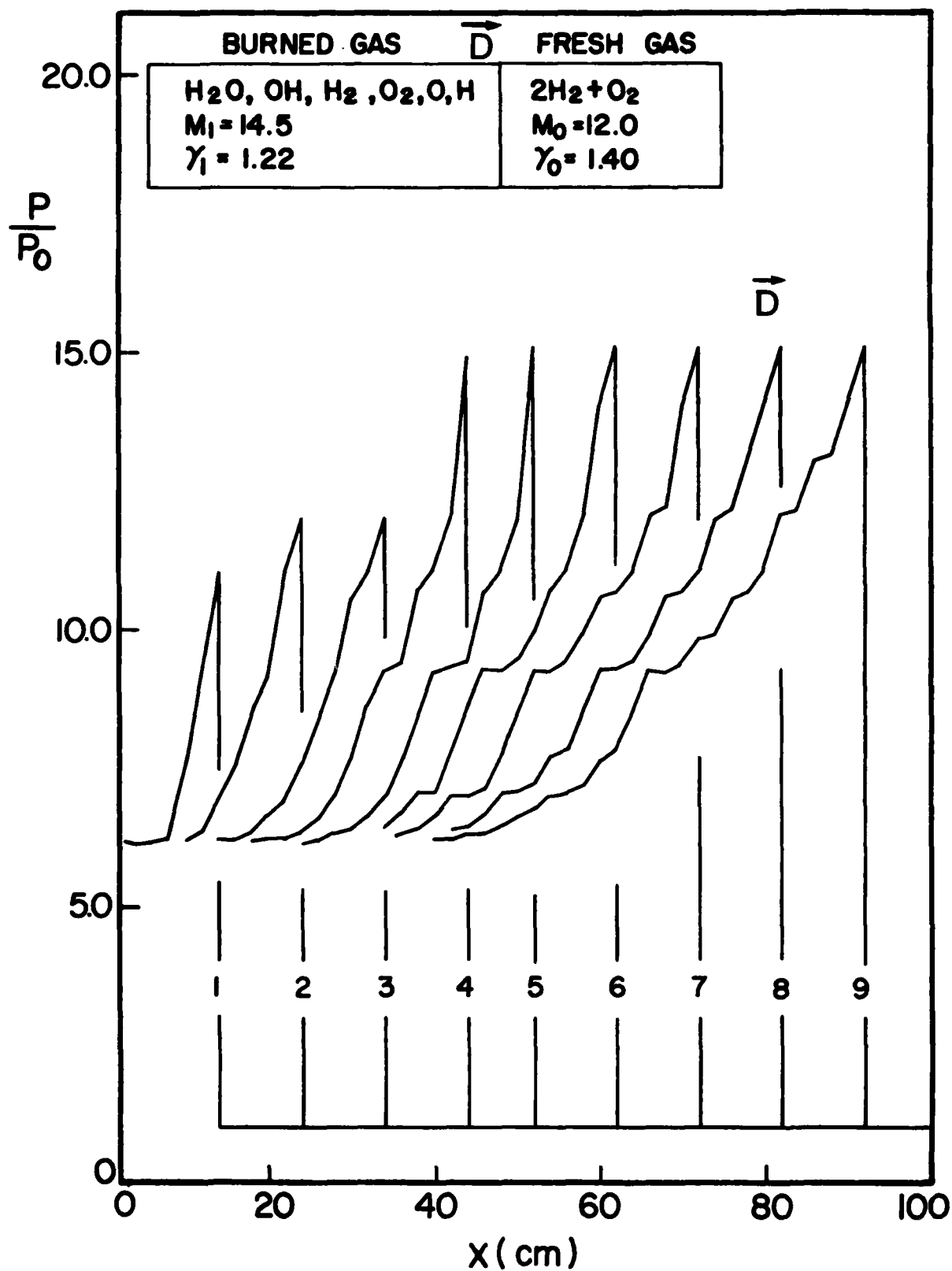


FIG. 20 PROPAGATION OF A DETONATION WAVE (D) IN A MIXTURE OF  $2H_2 + O_2$ . TIME NUMBERS: 1 - 41.1  $\mu s$ , 2 - 81.7  $\mu s$ , 3 - 122.  $\mu s$ , 4 - 162.  $\mu s$ , 5 - 202  $\mu s$ , 6 - 242  $\mu s$ , 7 - 282.  $\mu s$ , 8 - 322.  $\mu s$ , 9 - 362.  $\mu s$ .

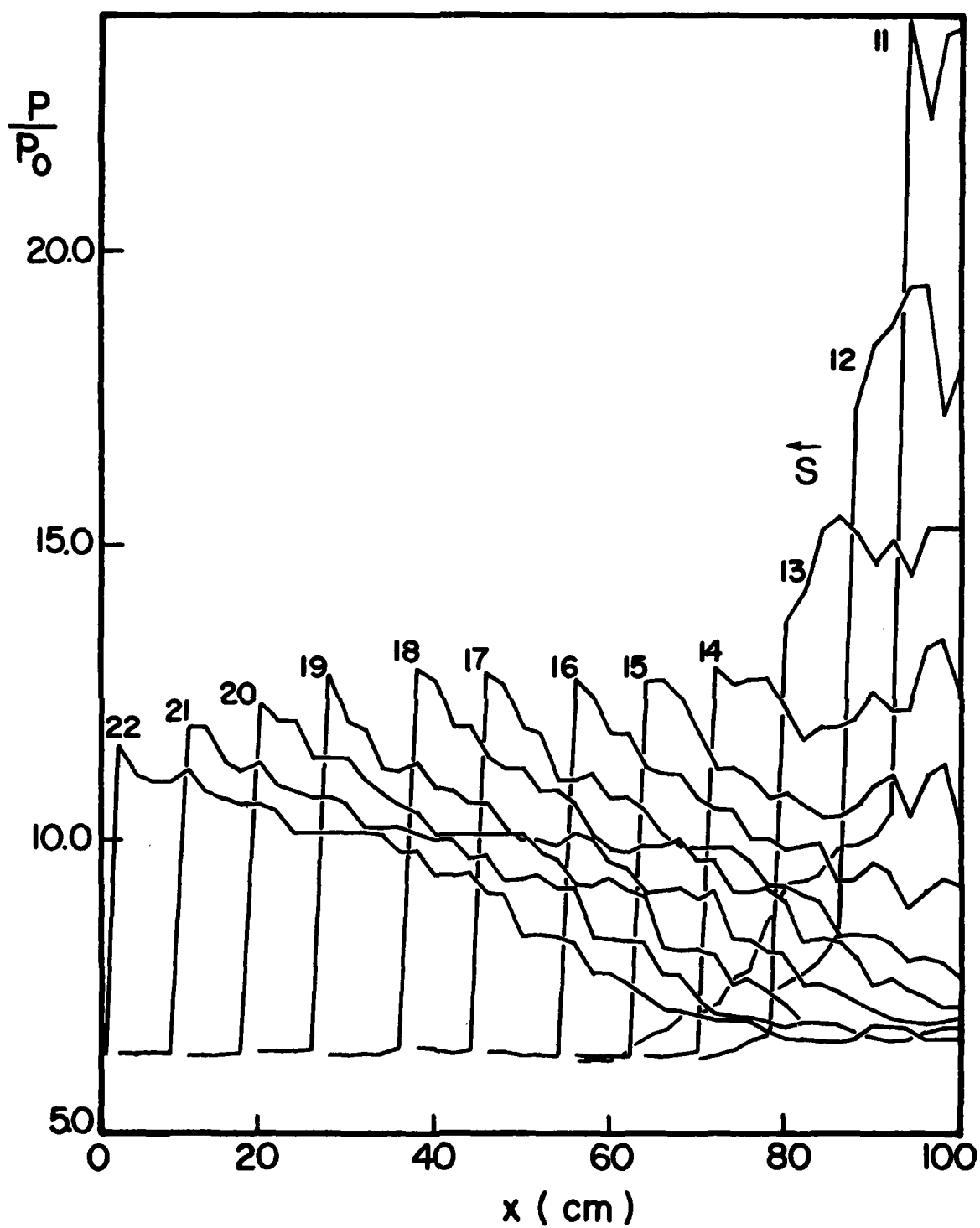


FIG. 21 REFLECTION OF A DETONATION WAVE IN  $2H_2 + O_2$  AT THE END WALL OF A TUBE.  
 TIME NUMBERS: 11 - 445.  $\mu s$ , 12 - 498.  $\mu s$ , 13 - 548.  $\mu s$ , 14 - 592.  $\mu s$ ,  
 15 - 637.  $\mu s$ , 16 - 681.  $\mu s$ , 17 - 725.  $\mu s$ , 18 - 770.  $\mu s$ , 19 - 816.  $\mu s$ ,  
 20 - 863.  $\mu s$ , 21 - 911.  $\mu s$ , 22 - 958.  $\mu s$ .

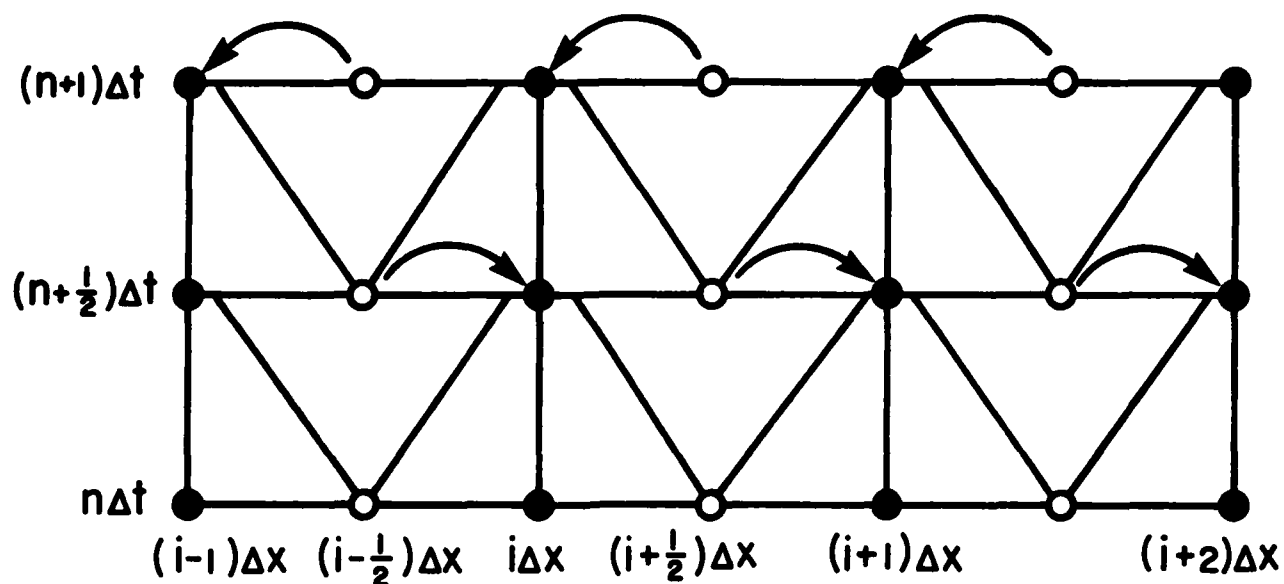


FIG. A-1-a COMPUTATIONAL DOMAIN. ● : ACTUAL GRID POINT; ○ : IMAGINARY GRID POINT.

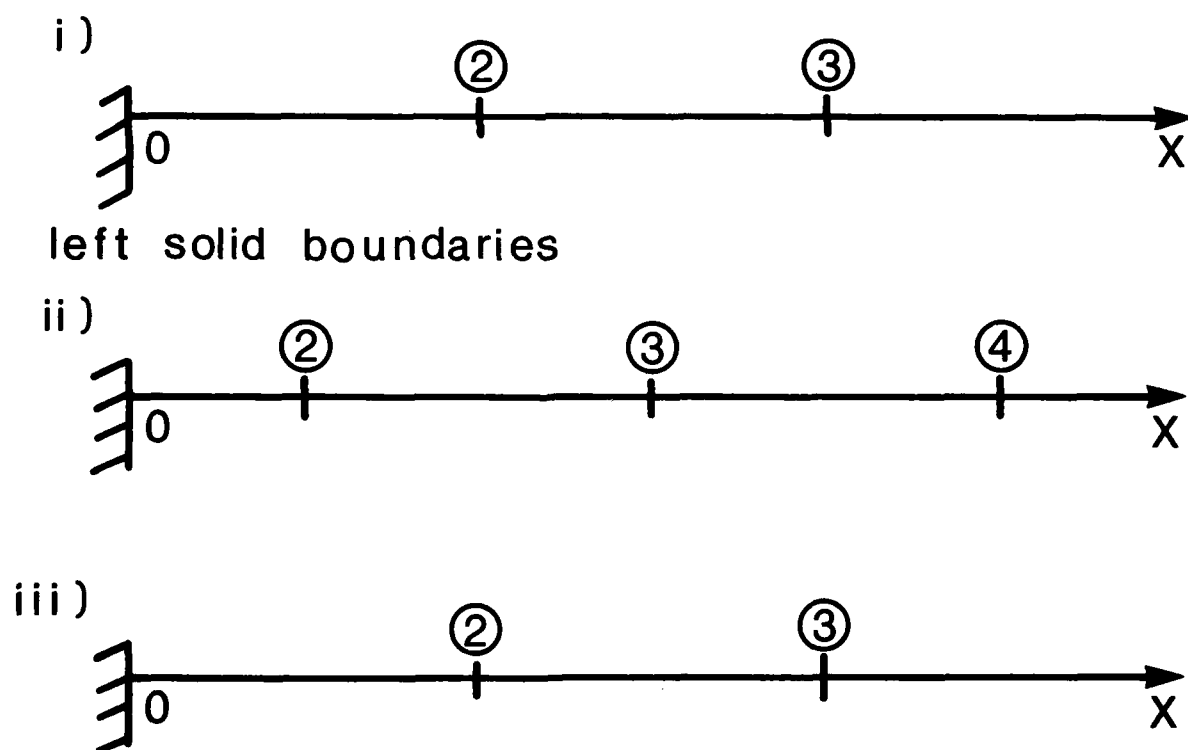


FIG. A-1-b RELATIONSHIP BETWEEN COMPUTATIONAL MESH POINTS AND ACTUAL PHYSICAL LOCATIONS. (i) WHEN CALCULATION STARTS, (ii) AFTER FIRST-HALF-STEP, (iii) AFTER SECOND-HALF-STEP. ②, ③, ... : CORRESPOND MESH POINTS.

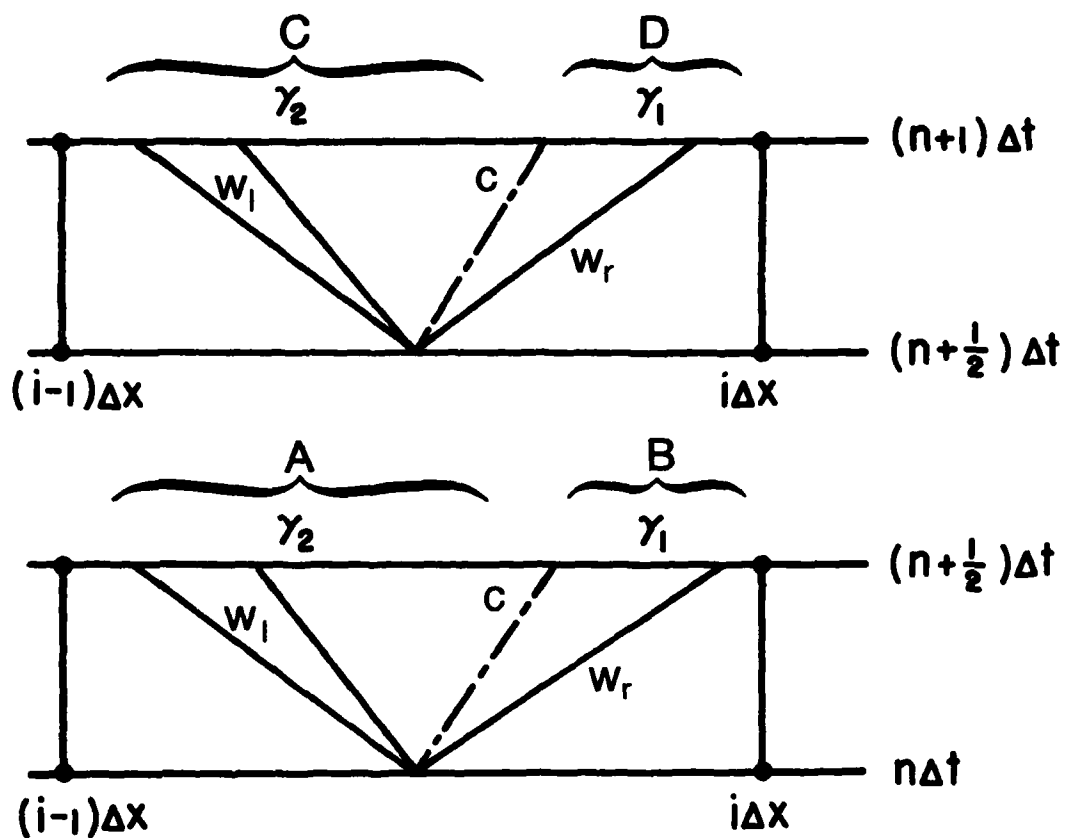


FIG. A-2 FOUR REGIONS WHICH DETERMINE MOVEMENT IN CONTACT SURFACE.  
 (i) IN FIRST-HALF STEP, (ii) IN SECOND-HALF STEP.



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APPLICATIONS OF RANDOM-CHOICE METHOD TO PROBLEMS IN SHOCK AND DETONATION-WAVE DYNAMICS

Saito, T., Glass, I. I.

1. Numerical Methods, 2. Shock waves, 3. Contact surfaces, 4. Rarefaction waves,
5. Blast waves, 6. Detonation waves

I. Saito, T., Glass, I. I. II. UTIAS Report No. 240

Although successful numerical methods exist for solving problems in shock and detonation-wave dynamics, there is still a real need of developing new techniques where the old methods fail to predict important flow properties. For example, it has recently been shown in Ref. 1 that existing methods fail to predict the intermetrically measured isopycnics in regular and single Mach reflections (let alone complex and double-Mach reflections), for which numerical solutions do not even exist. The purpose of the present report is to present eight applications of the Random-Choice Method (RCM) to the solution of problems in shock and detonation-wave dynamics. It is shown that unlike other numerical methods, the RCM yields sharp-fronted shocks and contact surfaces without resorting to artificial and perhaps erroneous means of predicting their locations, which depend more on art than science. It is also a very useful method in showing such fine points as the birth point of the second shock (implosion) wave at the tail of the rarefaction wave in a spherical explosion.

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